

# **STIC Search Report**

**EIC 1700**

**STIC Database Tracking Number: 182905**

**TO: Eisa Elhilo  
Location: REM 9A60  
Art Unit : 1751  
March 22, 2006**

**Case Serial Number: 10/807162**

**From: Les Henderson  
Location: EIC 1700  
REM 4B28 / 4A30  
Phone: 571-272-2538**

**Leslie.henderson@uspto.gov**

## **Search Notes**



# STIC Search Results Feedback Form

**EIC17000**

Questions about the scope or the results of the search? Contact *the EIC searcher or contact:*

Kathleen Fuller, EIC 1700 Team Leader  
571/272-2505 REMSEN 4B28

## Voluntary Results Feedback Form

- I am an examiner in Workgroup:  Example: 1713  
➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature  
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28

=> d his

(FILE 'HOME' ENTERED AT 14:38:21 ON 22 MAR 2006)

FILE 'HCAPLUS' ENTERED AT 14:38:33 ON 22 MAR 2006

L1 E US20050066451/PN  
1 S US20050066451/PN  
SEL RN

FILE 'REGISTRY' ENTERED AT 14:39:22 ON 22 MAR 2006

L2 47 S E1-E47

FILE 'LREGISTRY' ENTERED AT 14:44:12 ON 22 MAR 2006

L3 STR

FILE 'REGISTRY' ENTERED AT 14:48:45 ON 22 MAR 2006

L4 50 S L3

FILE 'LREGISTRY' ENTERED AT 14:49:22 ON 22 MAR 2006

L5 STR L3

FILE 'REGISTRY' ENTERED AT 14:49:56 ON 22 MAR 2006

L6 50 S L5

FILE 'LREGISTRY' ENTERED AT 14:54:16 ON 22 MAR 2006

L7 STR L5

FILE 'REGISTRY' ENTERED AT 14:55:06 ON 22 MAR 2006

L8 38 S L7

L9 846 S L7 FUL

SAV L9 ELH162/A

L10 34 S L2 AND L9

FILE 'LREGISTRY' ENTERED AT 15:02:14 ON 22 MAR 2006

L11 STR L7

FILE 'REGISTRY' ENTERED AT 15:04:12 ON 22 MAR 2006

L12 9 S L11 SSS SAM SUB=L9

L13 207 S L11 SSS FUL SUB=L9

SAV L13 ELH162A/A

L14 34 S L13 AND L2

FILE 'HCAPLUS' ENTERED AT 15:06:56 ON 22 MAR 2006

L15 1 S L14

L16 63 S L13

L17 454 S L9

L18 1 S L15 AND L16

L19 7778 S HAIR?(2N) (DYE? OR DY? OR COLOR? OR COLOUR?)

L20 3 S L16 AND L19

L21 4 S L17 AND L19

L22 2019 S KERA?(2N) (FIBER OR FIBRE)

L23 3 S L16 AND L22

L24 3 S L22 AND L17

L25 162443 S COSMET?/SC,SX

L26 3 S L25 AND L16

L27 5 S L25 AND L17

FILE 'LREGISTRY' ENTERED AT 15:14:07 ON 22 MAR 2006

L28 STR L11

FILE 'REGISTRY' ENTERED AT 15:19:23 ON 22 MAR 2006

L29 8 S L28 SSS SAM SUB=L9

L30 243 S L28 SSS FUL SUB=L9

SAV L30 ELH162B/A

L31 8 S L28 SSS SAM SUB=L13

L32 199 S L28 SSS FUL SUB=L13

L33 34 S L32 AND L2  
 L34 34 S L30 AND L2  
 SAV L32 ELH162C/A

FILE 'HCAPLUS' ENTERED AT 15:23:31 ON 22 MAR 2006

L35 86 S L30  
 L36 86 S L35  
 L37 86 S L35 OR L36  
 L38 3 S L37 AND (L19 OR L22 OR L25)  
 L39 1176472 S DY?  
 L40 7 S L37 AND L39  
 L41 4 S L40 AND (DYSTROPH? OR DYSFUNC? OR DYSLIP?)  
 L42 3 S L40 NOT L41  
 L43 5 S L20 OR L23 OR L24 OR L26 OR L27 OR L38 OR L42  
 L44 60 S L16 NOT L43

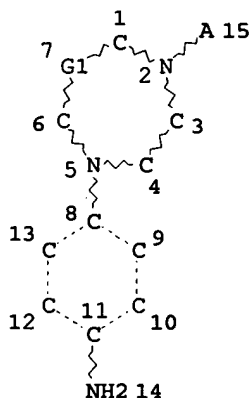
FILE 'CAOLD' ENTERED AT 15:33:29 ON 22 MAR 2006

L45 1 S L16  
 L46 2 S L30  
 L47 6 S L9  
 L48 6 S L45-L47

FILE 'HCAPLUS' ENTERED AT 15:39:05 ON 22 MAR 2006

L49 161083 S DYE?/SC,SX  
 L50 1 S L49 AND L37  
 L51 1 S L50 AND L17  
 L52 5 S L43 OR L50 OR L51

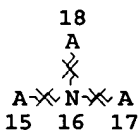
=> d que stat l52  
 L7 STR



REP G1=(0-1) C  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

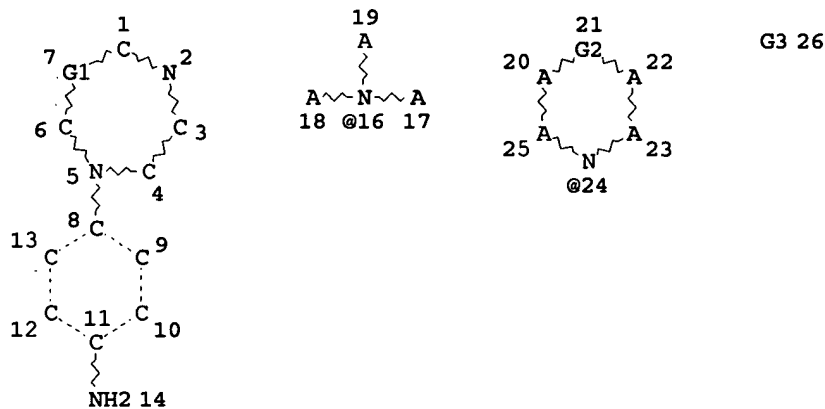
GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE  
 L9 846 SEA FILE=REGISTRY SSS FUL L7  
 L11 STR



STEREO ATTRIBUTES: NONE.

L13	207	SEA	FILE=REGISTRY	SUB=L9	SSS	FUL	L11
L16	63	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L13
L17	454	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L9
L19	7778	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	HAIR?	(2A) (DYE? OR DY?
						OR COLOR? OR COLOUR?)	
L20	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L16 AND L19
L22	2019	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	KERA?	(2A) (FIBER OR
						FIBRE)	
L23	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L16 AND L22
L24	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L22 AND L17
L25	162443	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	COSMET?/SC, SX	
L26	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L25 AND L16
L27	5	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON		L25 AND L17
L28		STR					



571-272-2538

NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L30 243 SEA FILE=REGISTRY SUB=L9 SSS FUL L28  
L35 86 SEA FILE=HCAPLUS ABB=ON PLU=ON L30  
L36 86 SEA FILE=HCAPLUS ABB=ON PLU=ON L30  
L37 86 SEA FILE=HCAPLUS ABB=ON PLU=ON L35 OR L36  
L38 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 AND (L19 OR L22  
OR L25)  
L39 1176472 SEA FILE=HCAPLUS ABB=ON PLU=ON DY?  
L40 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 AND L39  
L41 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L40 AND (DYSTROPH? OR  
DYSFUNC? OR DYSLIP?)  
L42 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L40 NOT L41  
L43 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 OR L23 OR L24 OR  
L26 OR L27 OR L38 OR L42  
L49 161083 SEA FILE=HCAPLUS ABB=ON PLU=ON DYE?/SC,SX  
L50 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND L37  
L51 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 AND L17  
L52 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 OR L50 OR L51

=> d l52 1-5 ibib abs hitstr hitind

L52 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1079846 HCAPLUS  
DOCUMENT NUMBER: 142:62280  
TITLE: p-Phenylenediamine derivatives comprising a  
diazacycloheptane ring as hair dyes  
INVENTOR(S): Sabelle, Stephane; Leduc, Madeleine; Ramos,  
Stanbury Laure  
PATENT ASSIGNEE(S): L'Oreal, Fr.  
SOURCE: Fr. Demande, 38 pp.  
CODEN: FRXXBL  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2856059	A1	20041217	FR 2003-7165	2003 0613
FR 2856059	B1	20051028		
WO 2004111062	A1	20041223	WO 2004-EP7192	2004 0611

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ,  
CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG,  
ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,  
KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,  
MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL,  
PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR,  
TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM,  
ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH,  
CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,  
MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI,

CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 PRIORITY APPLN. INFO.: FR 2003-7165

A  
 2003  
 0613

OTHER SOURCE(S): MARPAT 142:62280

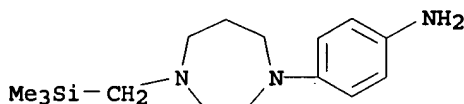
AB The invention relates to a p-phenylenediamine derivative comprising a diazacycloheptane ring with silyl groups for hair dyeing. Thus, 4-{4-[3-(trimethylsilyl)propyl]-1,4-diazepan-1-yl}phenylamine-HCl (I) was prepared by the reaction of 1-(4-nitrophenyl)-1,4-diazepan with 3-(trimethylsilyl)propyl chloride followed by Pd/C reduction. A formulation contained 10-3 mol I and 10-3 2-methyl-5-aminophenol in addition to the standard hair dye formulation components.

IT 808110-78-3 808110-79-4 808110-80-7  
 808110-81-8 808110-82-9 808110-83-0  
 808110-84-1 808110-85-2 808110-86-3  
 808110-87-4 808110-88-5 808110-89-6  
 808110-90-9 808110-91-0 808110-92-1  
 808110-93-2 808110-94-3 808110-95-4  
 808110-96-5 808110-97-6 808110-98-7

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
 (phenylenediamine derivs. comprising diazacycloheptane ring as hair dyes)

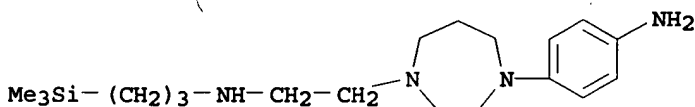
RN 808110-78-3 HCAPLUS

CN Benzenamine, 4-[hexahydro-4-[(trimethylsilyl)methyl]-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)



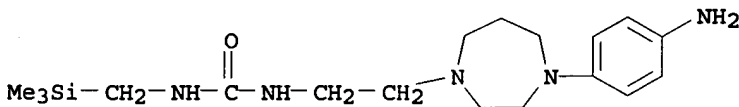
RN 808110-79-4 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanamine, 4-(4-aminophenyl)hexahydro-N-[3-(trimethylsilyl)propyl]- (9CI) (CA INDEX NAME)



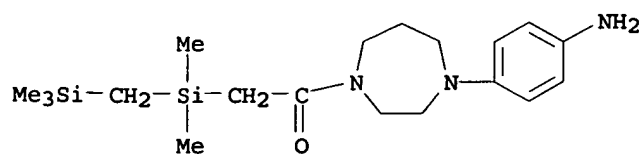
RN 808110-80-7 HCAPLUS

CN Urea, N-[2-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-yl]ethyl]-N'-[(trimethylsilyl)methyl]- (9CI) (CA INDEX NAME)

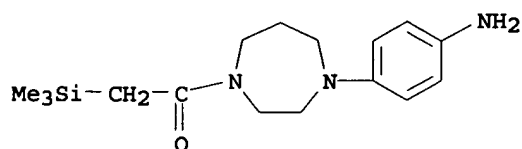


RN 808110-81-8 HCAPLUS

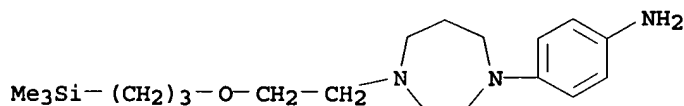
CN 1H-1,4-Diazepine, 1-(4-aminophenyl)-4-[[dimethyl[(trimethylsilyl)methyl]silyl]acetyl]hexahydro- (9CI) (CA INDEX NAME)



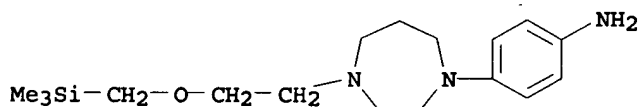
RN 808110-82-9 HCAPLUS  
 CN 1H-1,4-Diazepine, 1-(4-aminophenyl)hexahydro-4-  
 [(trimethylsilyl)acetyl]- (9CI) (CA INDEX NAME)



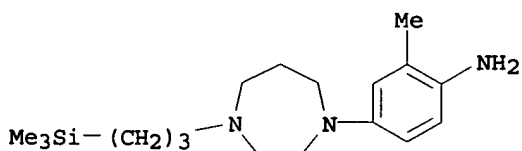
RN 808110-83-0 HCAPLUS  
 CN Benzenamine, 4-[hexahydro-4-[2-[3-(trimethylsilyl)propoxy]ethyl]-  
 1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)



RN 808110-84-1 HCAPLUS  
 CN Benzenamine, 4-[hexahydro-4-[2-[(trimethylsilyl)methoxy]ethyl]-1H-  
 1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

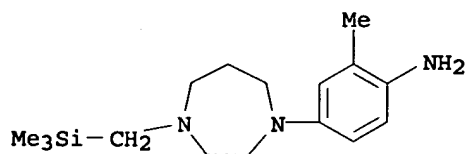


RN 808110-85-2 HCAPLUS  
 CN Benzenamine, 4-[hexahydro-4-[3-(trimethylsilyl)propyl]-1H-1,4-  
 diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)



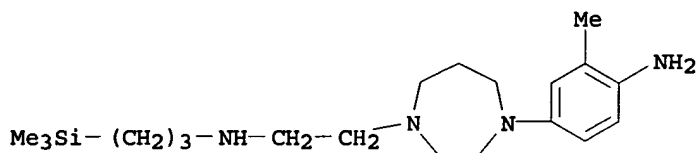
RN 808110-86-3 HCAPLUS  
 CN Benzenamine, 4-[hexahydro-4-[(trimethylsilyl)methyl]-1H-1,4-  
 diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)





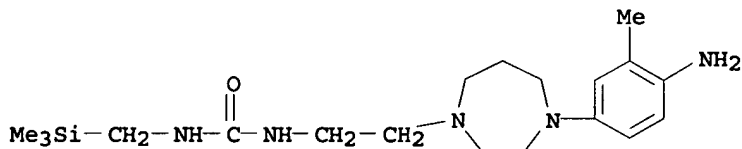
RN 808110-87-4 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanamine, 4-(4-amino-3-methylphenyl)hexahydro-  
N-[3-(trimethylsilyl)propyl]- (9CI) (CA INDEX NAME)



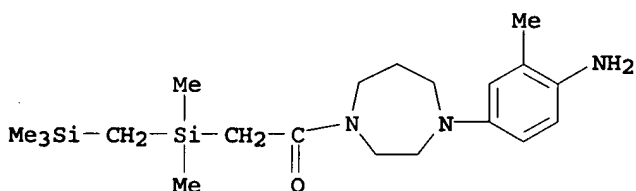
RN 808110-88-5 HCAPLUS

CN Urea, N-[2-[4-(4-amino-3-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]ethyl]-N'-[(trimethylsilyl)methyl]- (9CI) (CA INDEX NAME)



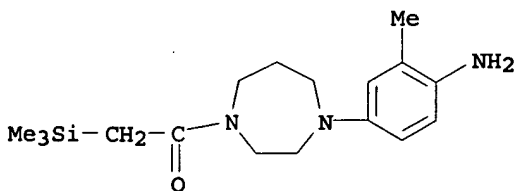
RN 808110-89-6 HCAPLUS

CN 1H-1,4-Diazepine, 1-(4-amino-3-methylphenyl)-4-  
[[dimethyl[(trimethylsilyl)methyl]silyl]acetyl]hexahydro- (9CI)  
(CA INDEX NAME)



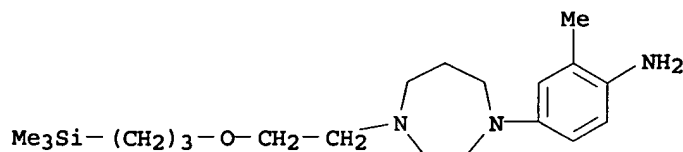
RN 808110-90-9 HCAPLUS

CN 1H-1,4-Diazepine, 1-(4-amino-3-methylphenyl)hexahydro-4-  
[(trimethylsilyl)acetyl]- (9CI) (CA INDEX NAME)



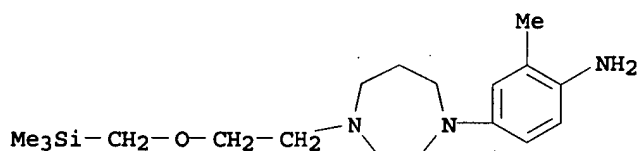
RN 808110-91-0 HCAPLUS

CN Benzenamine, 4-[hexahydro-4-[2-[3-(trimethylsilyl)propoxy]ethyl]-1H-1,4-diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)



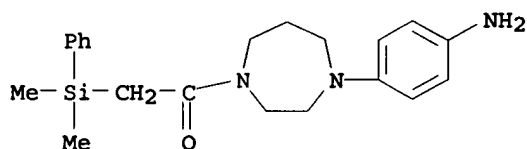
RN 808110-92-1 HCAPLUS

CN Benzenamine, 4-[hexahydro-4-[2-[(trimethylsilyl)methoxy]ethyl]-1H-1,4-diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)



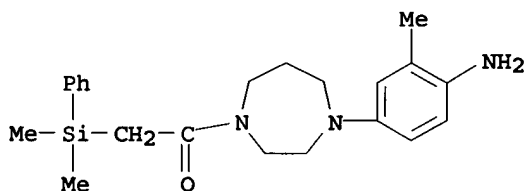
RN 808110-93-2 HCAPLUS

CN 1H-1,4-Diazepine, 1-(4-aminophenyl)-4-[(dimethylphenylsilyl)acetyl]hexahydro- (9CI) (CA INDEX NAME)



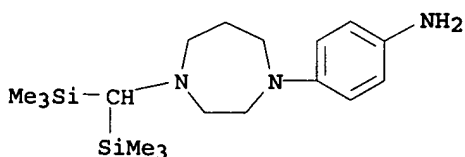
RN 808110-94-3 HCAPLUS

CN 1H-1,4-Diazepine, 1-(4-amino-3-methylphenyl)-4-[(dimethylphenylsilyl)acetyl]hexahydro- (9CI) (CA INDEX NAME)

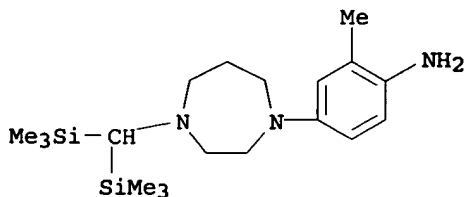


RN 808110-95-4 HCAPLUS

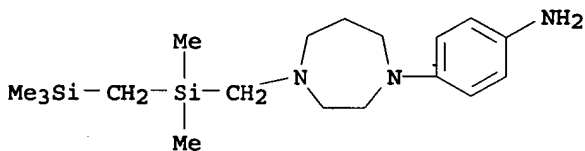
CN Benzenamine, 4-[4-[bis(trimethylsilyl)methyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)



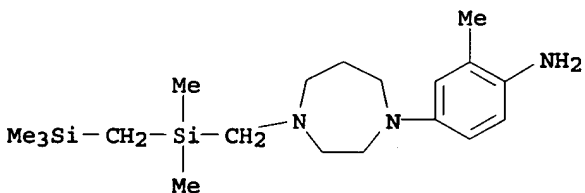
RN 808110-96-5 HCAPLUS  
 CN Benzenamine, 4-[4-[bis(trimethylsilyl)methyl]hexahydro-1H-1,4-diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)



RN 808110-97-6 HCAPLUS  
 CN Benzenamine, 4-[4-[[dimethyl[(trimethylsilyl)methyl]silyl]methyl]hexahydro-1H-1,4-diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)

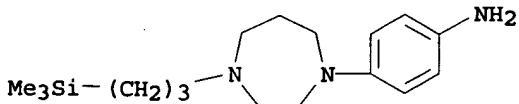


RN 808110-98-7 HCAPLUS  
 CN Benzenamine, 4-[4-[[dimethyl[(trimethylsilyl)methyl]silyl]methyl]hexahydro-1H-1,4-diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)

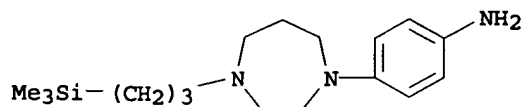


IT 808110-77-2P 808111-00-4P  
 RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (phenylenediamine derivs. comprising diazacycloheptane ring as hair dyes)

RN 808110-77-2 HCAPLUS  
 CN Benzenamine, 4-[hexahydro-4-[3-(trimethylsilyl)propyl]-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)



RN 808111-00-4 HCAPLUS  
 CN Benzenamine, 4-[hexahydro-4-[3-(trimethylsilyl)propyl]-1H-1,4-diazepin-1-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IC ICM C07D243-08  
ICS A61K007-13  
CC 62-3 (Essential Oils and Cosmetics)  
IT 95-54-5D, o-Phenylenediamine, derivs. 95-55-6D, o-Aminophenol, derivs. 108-45-2D, m-Phenylenediamine, derivs. 108-46-3, Resorcinol, biological studies 108-46-3D, Resorcinol, derivs. 123-30-8D, p-Aminophenol, derivs. 124-43-6 591-27-5D, m-Aminophenol, derivs. 2380-86-1, 6-Hydroxyindole 2835-95-2 7722-84-1, Hydrogen peroxide, biological studies 9035-73-8, Oxidase 16867-03-1, 2-Amino-3-hydroxypyridine 30569-52-9 66422-95-5 80419-48-3 808110-78-3 808110-79-4 808110-80-7 808110-81-8 808110-82-9 808110-83-0 808110-84-1 808110-85-2 808110-86-3 808110-87-4 808110-88-5 808110-89-6 808110-90-9 808110-91-0 808110-92-1 808110-93-2 808110-94-3 808110-95-4 808110-96-5 808110-97-6 808110-98-7  
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (phenylenediamine derivs. comprising diazacycloheptane ring as hair dyes)  
IT 808110-77-2P 808111-00-4P  
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (phenylenediamine derivs. comprising diazacycloheptane ring as hair dyes)  
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L52 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:796300 HCAPLUS

DOCUMENT NUMBER: 141:295850

TITLE: Preparation of p-phenylenediamines with a cyclic diaza group substituted by a cationic radical, and their use for dyeing keratinic fibers

INVENTOR(S): Sabelle, Stephane; Genet, Alain; Leduc, Madeleine

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 35 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1462445	A1	20040929	EP 2004-290723	

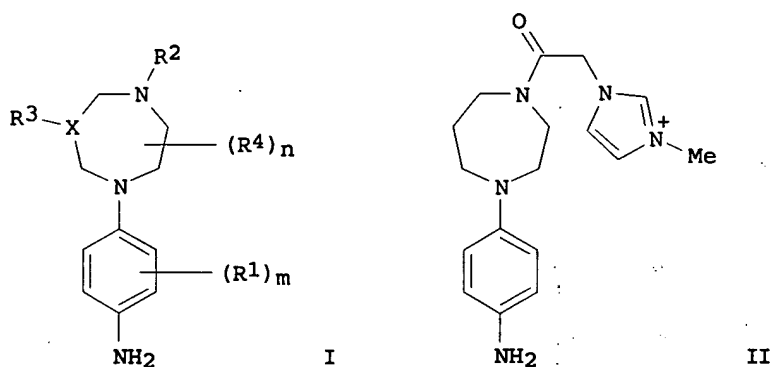
2004  
0317

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,

MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,  
EE, HU, PL, SK, HR

FR 2852955	A1	20041001	FR 2003-3548	2003 0324
JP 2004292448	A2	20041021	JP 2004-85683	2004 0323
US 2005066451	A1	20050331	US 2004-807162	2004 0324
PRIORITY APPLN. INFO.:			FR 2003-3548	A 2003 0324
			US 2003-467123P	P 2003 0502

OTHER SOURCE(S): MARPAT 141:295850  
GI



- AB Title compds. I [wherein X = (CH<sub>2</sub>)<sub>q</sub>; m = 0-4; when m ≥ 2, R<sub>1</sub> can be identical or different; n = 0-4; when n ≥ 2, R<sub>4</sub> can be identical or different; q = 0-1; R<sub>1</sub> = Z, halo, (un)saturated aliphatic or alicyclic hydrocarbonyl with at least one carbon replaced by O, N, Si, S, SO<sub>2</sub>; R<sub>2</sub> = Z; R<sub>3</sub> = alkenyl, alkynyl, hydroxy/alkoxy/hydroxyalkoxy/amino/carboxy/carbamoyl/alkyl, OH, alkoxy, alkylcarbonyl, monoalkyl/dialkyl/amino, etc.; R<sub>4</sub> = alkenyl, alkynyl, hydroxy/alkoxy/hydroxyalkoxy//amino/carboxy/carbamoyl/alkyl, alkylcarbonyl, CO<sub>2</sub>H, carbamoyl, etc.; and their addition salts] were prepared as oxidation bases for **dyeing keratinous fibers**, in particular human hair fibers. For example, II•Cl•HCl was prepared by acylation of 1-(4-nitrophenyl)-1,4-diazepane with chloroacetyl chloride, amination of the chloride with 1-methyl-1H-imidazole, hydrogenation of the nitrophenyl intermediate over Pd/C, followed by acidulation with HCl. Formulations of II•Cl•HCl in acidic medium gave blue-violet and violet-gray shades.
- IT 765295-81-6P, 3-[2-[4-(4-Aminophenyl)-1,4-diazepan-1-yl]-2-oxoethyl]-1-methyl-3H-imidazol-1-ium chloride dihydrochloride  
765295-83-8P 765295-84-9P 765295-85-0P  
765295-86-1P 765295-87-2P 765295-88-3P  
765295-89-4P 765295-90-7P 765295-91-8P  
765295-92-9P 765295-93-0P 765295-94-1P  
765295-95-2P 765295-96-3P 765295-97-4P

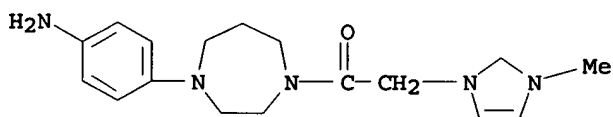
765295-98-5P 765295-99-6P 765296-00-2P  
 765296-01-3P 765296-02-4P 765296-03-5P  
 765296-04-6P 765296-05-7P 765296-06-8P  
 765296-07-9P 765296-08-0P 765296-09-1P  
 765296-10-4P 765296-11-5P 765296-12-6P  
 765296-13-7P 765296-14-8P 765296-21-7P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation); USES (Uses)

(oxidation base for **dyeing**; preparation of  
 p-phenylenediamines with a cyclic diaza group substituted by a  
 cationic radical, and their use for **dyeing**  
**keratinic fibers**)

RN 765295-81-6 HCAPLUS

CN 1H-Imidazolium, 1-[2-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-yl]-2-oxoethyl]-3-methyl-, chloride, dihydrochloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

● 2 HCl

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

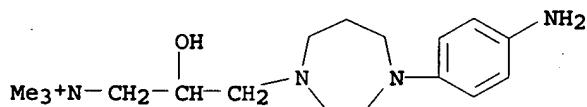
RN 765295-83-8 HCAPLUS

CN 1H-1,4-Diazepine-1-propanaminium, 4-(4-aminophenyl)hexahydro-β-hydroxy-N,N,N-trimethyl-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 765295-82-7

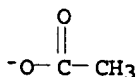
CMF C17 H31 N4 O



CM 2

CRN 71-50-1

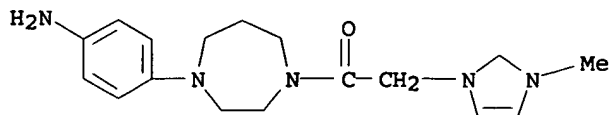
CMF C2 H3 O2



RN 765295-84-9 HCAPLUS

CN 1H-Imidazolium, 1-[2-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-

yl]-2-oxoethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

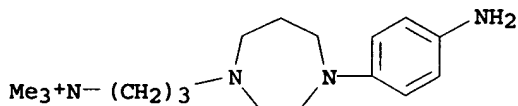


● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765295-85-0 HCAPLUS

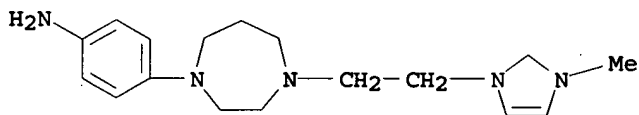
CN 1H-1,4-Diazepine-1-propanaminium, 4-(4-aminophenyl)hexahydro-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 765295-86-1 HCAPLUS

CN 1H-Imidazolium, 1-[2-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-yl]ethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

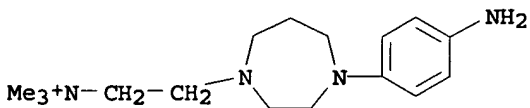


● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765295-87-2 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanaminium, 4-(4-aminophenyl)hexahydro-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)

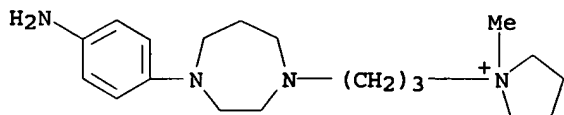


● Cl<sup>-</sup>

RN 765295-88-3 HCAPLUS

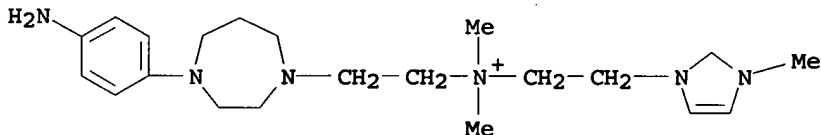
CN Pyrrolidinium, 1-[3-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-

ylpropyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

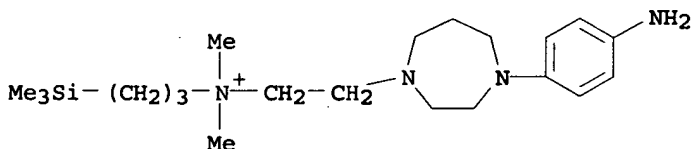
RN 765295-89-4 HCAPLUS  
 CN 1H-Imidazolium, 1-[2-[[2-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-yl]ethyl]dimethylammonio]ethyl]-3-methyl-, dichloride (9CI) (CA INDEX NAME)



● 2 Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

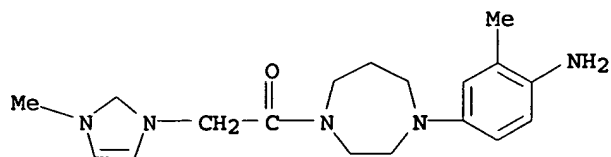
RN 765295-90-7 HCAPLUS  
 CN 1H-1,4-Diazepine-1-ethanaminium, 4-(4-aminophenyl)hexahydro-N,N-dimethyl-N-[3-(trimethylsilyl)propyl]-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 765295-91-8 HCAPLUS  
 CN 1H-Imidazolium, 1-[2-[4-(4-amino-3-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]-2-oxoethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

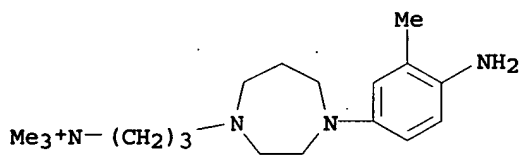


● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

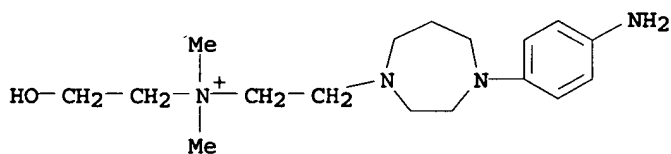
RN 765295-92-9 HCAPLUS

CN 1H-1,4-Diazepine-1-propanaminium, 4-(4-amino-3-methylphenyl)hexahydro-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

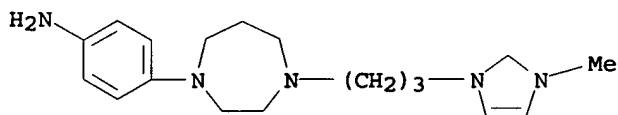
RN 765295-93-0 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanaminium, 4-(4-aminophenyl)hexahydro-N-(2-hydroxyethyl)-N,N-dimethyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

RN 765295-94-1 HCAPLUS

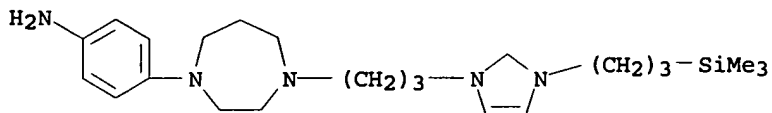
CN 1H-Imidazolium, 1-[3-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-yl]propyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765295-95-2 HCAPLUS

CN 1H-Imidazolium, 1-[3-[4-(4-aminophenyl)hexahydro-1H-1,4-diazepin-1-yl]propyl]-3-[3-(trimethylsilyl)propyl]-, chloride (9CI) (CA INDEX NAME)

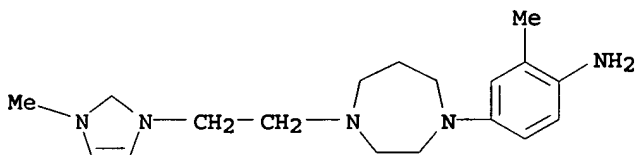


● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765295-96-3 HCAPLUS

CN 1H-Imidazolium, 1-[2-[4-(4-amino-3-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]ethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

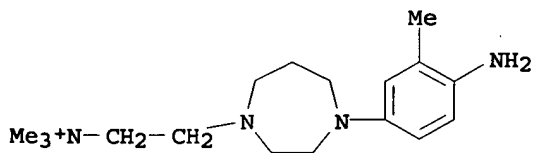


● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765295-97-4 HCAPLUS

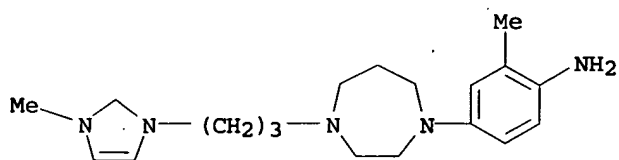
CN 1H-1,4-Diazepine-1-ethanaminium, 4-(4-amino-3-methylphenyl)hexahydro-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 765295-98-5 HCAPLUS

CN 1H-Imidazolium, 1-[3-[4-(4-amino-3-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]propyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

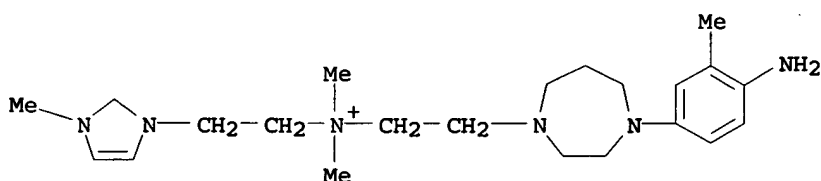


● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765295-99-6 HCAPLUS

CN 1H-Imidazolium, 1-[2-[[2-[4-(4-amino-3-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]ethyl]dimethylammonio]ethyl]-3-methyl-, dichloride (9CI) (CA INDEX NAME)

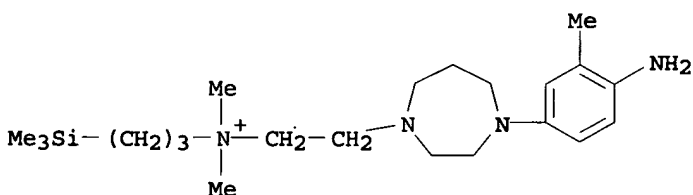


●2 Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765296-00-2 HCAPLUS

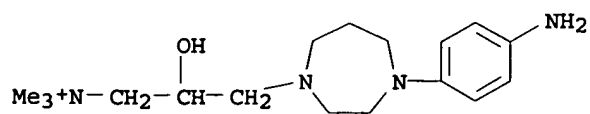
CN 1H-1,4-Diazepine-1-ethanaminium, 4-(4-amino-3-methylphenyl)hexahydro-N,N-dimethyl-N-[3-(trimethylsilyl)propyl]-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

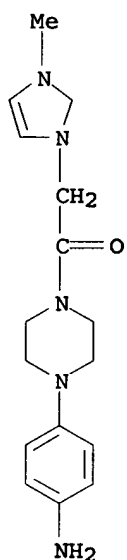
RN 765296-01-3 HCAPLUS

CN 1H-1,4-Diazepine-1-propanaminium, 4-(4-aminophenyl)hexahydro-β-hydroxy-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

RN 765296-02-4 HCAPLUS

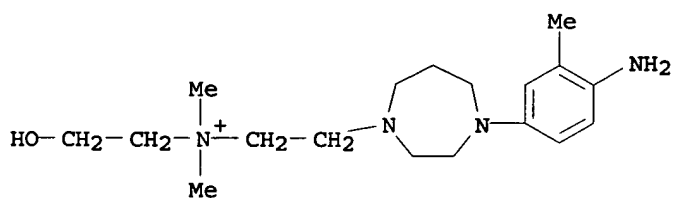
CN 1H-Imidazolium, 1-[2-[4-(4-aminophenyl)-1-piperazinyl]-2-oxoethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

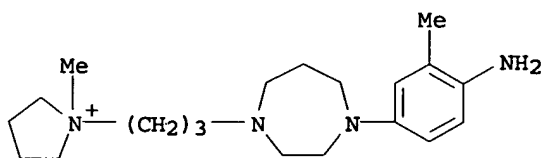
RN 765296-03-5 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanaminium, 4-(4-amino-3-methylphenyl)hexahydro-N-(2-hydroxyethyl)-N,N-dimethyl-, chloride (9CI) (CA INDEX NAME)

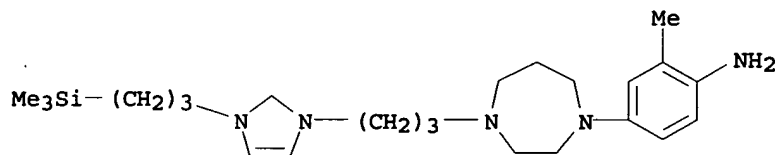
● Cl<sup>-</sup>

RN 765296-04-6 HCAPLUS

CN Pyrrolidinium, 1-[3-[4-(4-amino-3-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]propyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

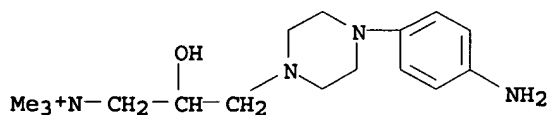
● Cl<sup>-</sup>

RN 765296-05-7 HCAPLUS  
 CN 1H-Imidazolium, 1-[3-[4-(4-amino-3-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]propyl]-3-[3-(trimethylsilyl)propyl]-, chloride (9CI) (CA INDEX NAME)

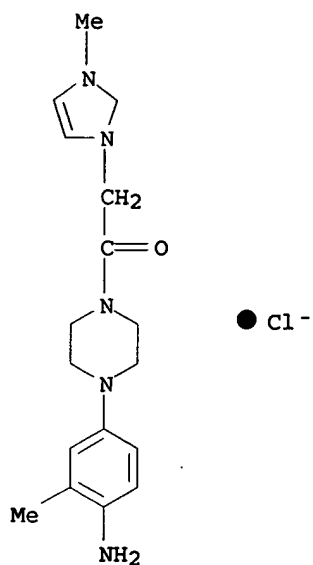
● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765296-06-8 HCAPLUS  
 CN 1-Piperazinepropanaminium, 4-(4-aminophenyl)-β-hydroxy-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

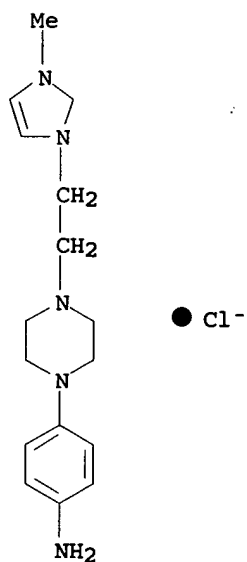
RN 765296-07-9 HCAPLUS  
 CN 1H-Imidazolium, 1-[2-[4-(4-amino-3-methylphenyl)-1-piperazinyl]-2-oxoethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765296-08-0 HCAPLUS

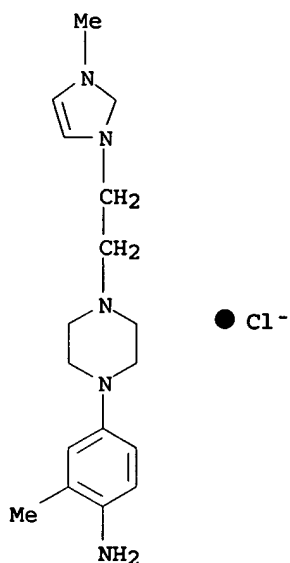
CN 1H-Imidazolium, 1-[2-[4-(4-aminophenyl)-1-piperazinyl]ethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 765296-09-1 HCAPLUS

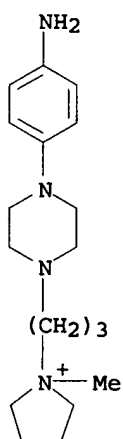
CN 1H-Imidazolium, 1-[2-[4-(4-amino-3-methylphenyl)-1-piperazinyl]ethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

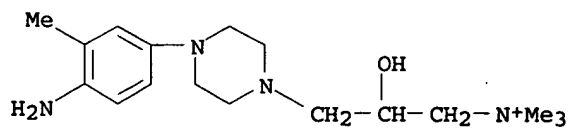
RN 765296-10-4 HCAPLUS

CN Pyrrolidinium, 1-[3-[4-(4-aminophenyl)-1-piperazinyl]propyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



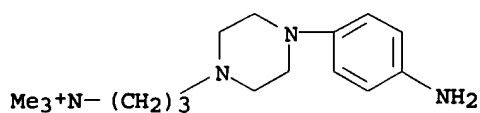
RN 765296-11-5 HCAPLUS

CN 1-Piperazinepropanaminium, 4-(4-amino-3-methylphenyl)-β-hydroxy-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



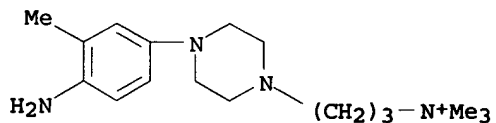
●  $\text{Cl}^-$

RN 765296-12-6 HCAPLUS  
 CN 1-Piperazinepropanaminium, 4-(4-aminophenyl)-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



●  $\text{Cl}^-$

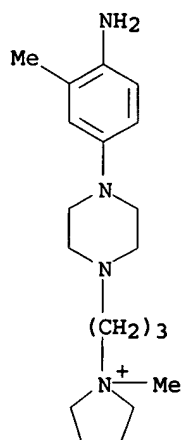
RN 765296-13-7 HCAPLUS  
 CN 1-Piperazinepropanaminium, 4-(4-amino-3-methylphenyl)-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



●  $\text{Cl}^-$

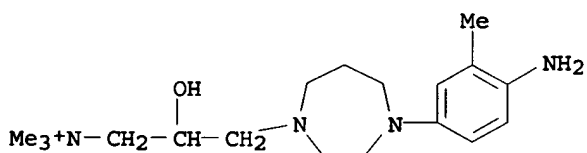
RN 765296-14-8 HCAPLUS  
 CN Pyrrolidinium, 1-[3-[4-(4-amino-3-methylphenyl)-1-piperazinyl]propyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)





● Cl<sup>-</sup>

RN 765296-21-7 HCAPLUS  
 CN 1H-1,4-Diazepine-1-propanaminium, 4-(4-amino-3-methylphenyl)hexahydro-β-hydroxy-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

IC ICM C07D233-54  
 ICS C07D243-06; C07D295-12; C07D403-12; A61K007-13  
 CC 27-10 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 62  
 ST diazepan phenylenediamine prepn hair dye  
 keratin fiber  
 IT Bromates  
 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
 (oxidizing agents; alkali metal; preparation of p-phenylenediamines with a cyclic diaza group substituted by a cationic radical, and their use for dyeing keratinic fibers)  
 IT Peroxy acids  
 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
 (oxidizing agents; preparation of p-phenylenediamines with a cyclic diaza group substituted by a cationic radical, and their use for dyeing keratinic fibers)  
 IT Hair preparations  
 Human  
 (preparation of p-phenylenediamines with a cyclic diaza group substituted by a cationic radical, and their use for dyeing keratinic fibers)

- IT 2380-86-1, 1H-Indol-6-ol 2835-95-2, 2-Methyl-5-aminophenol  
16867-03-1, 2-Aminopyridin-3-ol 54557-79-8, 3,6-Dimethyl-1H-  
pyrazolo[5,1-c]-[1,2,4]triazole 66422-95-5, 2-(2,4-  
Diaminophenoxy)ethanol dihydrochloride 80419-48-3,  
3-Amino-2-chloro-6-methylphenol hydrochloride 765296-19-3,  
2-(2,4-Diaminophenoxy)ethanol acetate dihydrochloride  
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(coupling agent; preparation of p-phenylenediamines with a cyclic  
diaz group substituted by a cationic radical, and their use  
for dyeing keratinic fibers)
- IT 765296-15-9P, 2-Chloro-1-[4-(4-nitrophenyl)-1,4-diazepan-1-  
yl]ethanone 765296-16-0P 765296-18-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of p-phenylenediamines with a cyclic  
diaz group substituted by a cationic radical, and their use  
for dyeing keratinic fibers)
- IT 765295-81-6P, 3-[2-[4-(4-Aminophenyl)-1,4-diazepan-1-yl]-2-  
oxoethyl]-1-methyl-3H-imidazol-1-ium chloride dihydrochloride  
765295-83-8P 765295-84-9P 765295-85-0P  
765295-86-1P 765295-87-2P 765295-88-3P  
765295-89-4P 765295-90-7P 765295-91-8P  
765295-92-9P 765295-93-0P 765295-94-1P  
765295-95-2P 765295-96-3P 765295-97-4P  
765295-98-5P 765295-99-6P 765296-00-2P  
765296-01-3P 765296-02-4P 765296-03-5P  
765296-04-6P 765296-05-7P 765296-06-8P  
765296-07-9P 765296-08-0P 765296-09-1P  
765296-10-4P 765296-11-5P 765296-12-6P  
765296-13-7P 765296-14-8P 765296-21-7P  
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL  
(Biological study); PREP (Preparation); USES (Uses)  
(oxidation base for dyeing; preparation of  
p-phenylenediamines with a cyclic diaz group substituted by a  
cationic radical, and their use for dyeing  
keratinic fibers)
- IT 616-47-7, 1-Methyl-1H-imidazole 34890-37-4,  
Glycidyltrimethylammonium acetate 214124-83-1,  
1-(4-Nitrophenyl)-1,4-diazepane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of p-phenylenediamines with a cyclic diaz group  
substituted by a cationic radical, and their use for  
dyeing keratinic fibers)

L52 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:794536 HCAPLUS

DOCUMENT NUMBER: 141:282418

TITLE: Composition for dyeing of  
keratinic fibers comprising  
a cationic derivative of p-phenylenediamine  
substituted by a diazacyclohexane or a  
diazacycloheptane

INVENTOR(S): Genet, Alain; Sabelle, Stephane

PATENT ASSIGNEE(S): L'oreal, Fr.

SOURCE: Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1462091	A1	20040929	EP 2004-290711	2004

0316

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,  
MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,  
EE, HU, PL, SK, HR

FR 2852830 A1 20041001 FR 2003-3547

2003  
0324

JP 2004285069 A2 20041014 JP 2004-85681

2004  
0323

US 2004237216 A1 20041202 US 2004-807167

2004  
0324

PRIORITY APPLN. INFO.:

FR 2003-3547

A

2003  
0324

US 2003-506766P

P

2003  
0930

OTHER SOURCE(S): MARPAT 141:282418

AB Compns. for dyeing of keratinic fibers

, e.g. hair, comprises an oxidation base, a cationic derivative of p-phenylenediamine substituted by a diazacyclohexane or a diazacycloheptane. 4-(4-Amino-phenyl)-1,1-dimethyl-[1,4]diazepan-1-ium, chloride, dihydrochloride (I) was prepared by hydrogenation of 1,1-dimethyl-4-(4-nitrophenyl) [1,4]diazepan-1-ium chloride in presence of Pd/C. A hair dye contained I 10-3, 2-(2,4-diamino-phenoxy)ethanol dihydrochloride 10-3, excipients and water q.s. 100 g.

IT 760975-61-9 760975-63-1 760975-66-4

760975-68-6 760975-70-0 760975-72-2

760975-74-4 760975-76-6 760975-78-8

760975-80-2 760975-82-4 760975-83-5

760975-84-6 760975-85-7 760975-86-8

760975-87-9 760975-88-0 760975-89-1

760975-90-4 760975-91-5 760975-92-6

760975-93-7 760975-94-8 760975-95-9

760975-96-0 760975-97-1 760975-98-2

760975-99-3

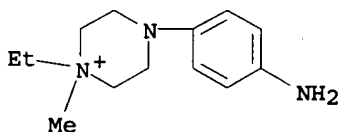
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(composition for dyeing of keratinic

fibers comprising cationic derivative of phenylenediamine substituted by diazacyclohexane or diazacycloheptane)

RN 760975-61-9 HCAPLUS

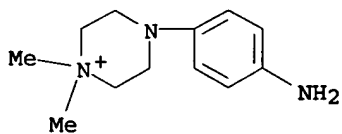
CN Piperazinium, 4-(4-aminophenyl)-1-ethyl-1-methyl-, chloride (9CI)  
(CA INDEX NAME)



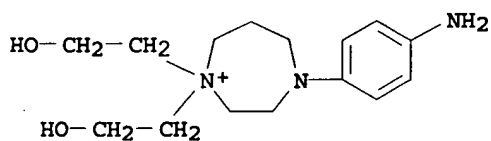
● Cl<sup>-</sup>

RN 760975-63-1 HCAPLUS

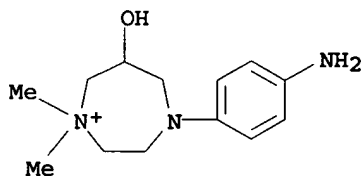
CN Piperazinium, 4-(4-aminophenyl)-1,1-dimethyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

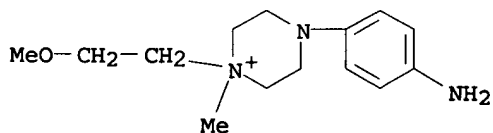
RN 760975-66-4 HCAPLUS  
 CN 1H-1,4-Diazepinium, 4-(4-aminophenyl)hexahydro-1,1-bis(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

RN 760975-68-6 HCAPLUS  
 CN 1H-1,4-Diazepinium, 4-(4-aminophenyl)hexahydro-6-hydroxy-1,1-dimethyl-, chloride (9CI) (CA INDEX NAME)

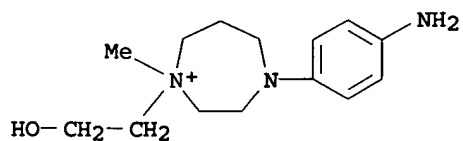
● Cl<sup>-</sup>

RN 760975-70-0 HCAPLUS  
 CN Piperazinium, 4-(4-aminophenyl)-1-(2-methoxyethyl)-1-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

RN 760975-72-2 HCAPLUS

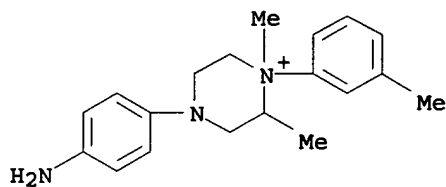
CN 1H-1,4-Diazepinium, 4-(4-aminophenyl)hexahydro-1-(2-hydroxyethyl)-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 760975-74-4 HCAPLUS

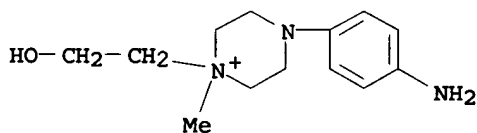
CN Piperazinium, 4-(4-aminophenyl)-1,2-dimethyl-1-(3-methylphenyl)-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 760975-76-6 HCAPLUS

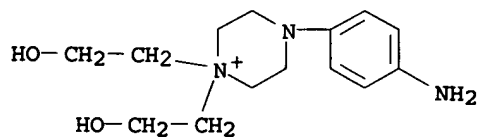
CN Piperazinium, 4-(4-aminophenyl)-1-(2-hydroxyethyl)-1-methyl-, chloride (9CI) (CA INDEX NAME)



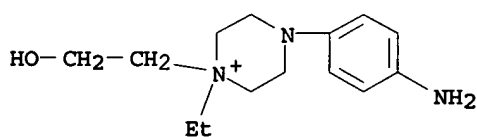
● Cl<sup>-</sup>

RN 760975-78-8 HCAPLUS

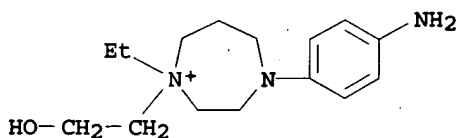
CN Piperazinium, 4-(4-aminophenyl)-1,1-bis(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

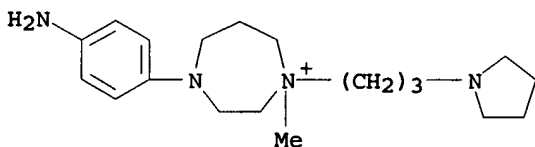
RN 760975-80-2 HCAPLUS  
 CN Piperazinium, 4-(4-aminophenyl)-1-ethyl-1-(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

RN 760975-82-4 HCAPLUS  
 CN 1H-1,4-Diazepinium, 4-(4-aminophenyl)-1-ethylhexahydro-1-(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)

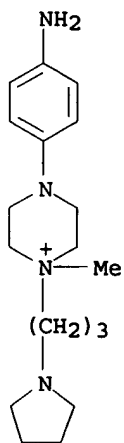
● Cl<sup>-</sup>

RN 760975-83-5 HCAPLUS  
 CN 1H-1,4-Diazepinium, 4-(4-aminophenyl)hexahydro-1-methyl-1-[3-(1-pyrrolidinyl)propyl]-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

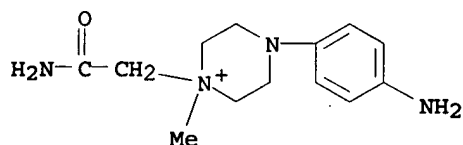
RN 760975-84-6 HCAPLUS  
 CN Piperazinium, 4-(4-aminophenyl)-1-methyl-1-[3-(1-

pyrrolidinyl)propyl]-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

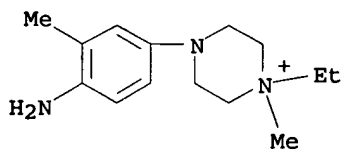
RN 760975-85-7 HCAPLUS

CN Piperazinium, 1-(2-amino-2-oxoethyl)-4-(4-aminophenyl)-1-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

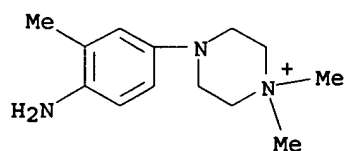
RN 760975-86-8 HCAPLUS

CN Piperazinium, 4-(4-amino-3-methylphenyl)-1-ethyl-1-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

RN 760975-87-9 HCAPLUS

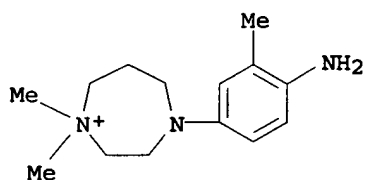
CN Piperazinium, 4-(4-amino-3-methylphenyl)-1,1-dimethyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 760975-88-0 HCAPLUS

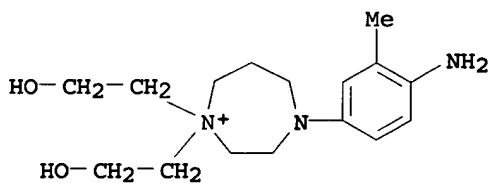
CN 1H-1,4-Diazepinium, 4-(4-amino-3-methylphenyl)hexahydro-1,1-dimethyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 760975-89-1 HCAPLUS

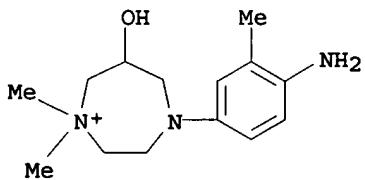
CN 1H-1,4-Diazepinium, 4-(4-amino-3-methylphenyl)hexahydro-1,1-bis(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 760975-90-4 HCAPLUS

CN 1H-1,4-Diazepinium, 4-(4-amino-3-methylphenyl)hexahydro-6-hydroxy-1,1-dimethyl-, chloride (9CI) (CA INDEX NAME)

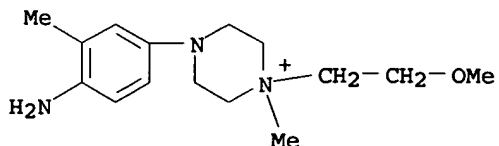


● Cl<sup>-</sup>



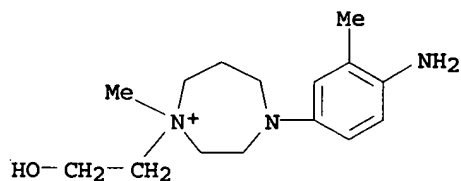
RN 760975-91-5 HCAPLUS

CN Piperazinium, 4-(4-amino-3-methylphenyl)-1-(2-methoxyethyl)-1-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

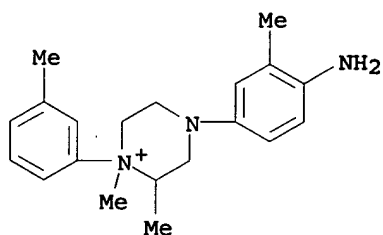
RN 760975-92-6 HCAPLUS

CN 1H-1,4-Diazepinium, 4-(4-amino-3-methylphenyl)hexahydro-1-(2-hydroxyethyl)-1-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

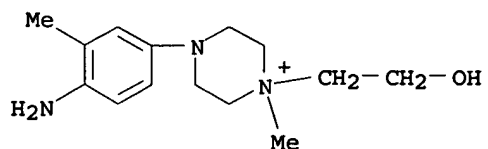
RN 760975-93-7 HCAPLUS

CN Piperazinium, 4-(4-amino-3-methylphenyl)-1,2-dimethyl-1-(3-methylphenyl)-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

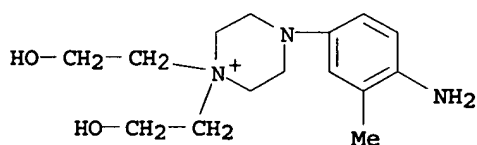
RN 760975-94-8 HCAPLUS

CN Piperazinium, 4-(4-amino-3-methylphenyl)-1-(2-hydroxyethyl)-1-methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

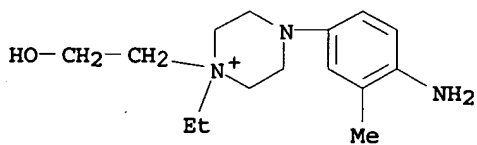
RN 760975-95-9 HCAPLUS

CN Piperazinium, 4-(4-amino-3-methylphenyl)-1,1-bis(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

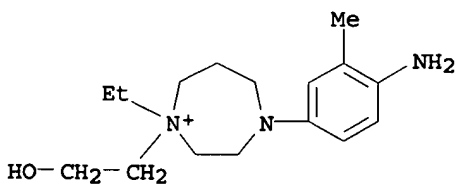
RN 760975-96-0 HCAPLUS

CN Piperazinium, 4-(4-amino-3-methylphenyl)-1-ethyl-1-(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)

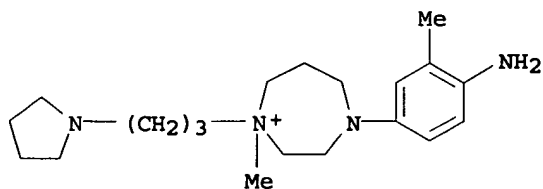
● Cl<sup>-</sup>

RN 760975-97-1 HCAPLUS

CN 1H-1,4-Diazepin-1-ium, 4-(4-amino-3-methylphenyl)-1-ethylhexahydro-1-(2-hydroxyethyl)-, chloride (9CI) (CA INDEX NAME)

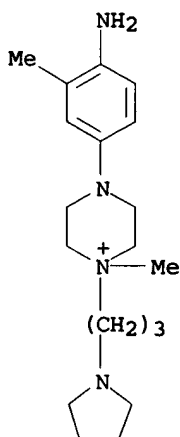
● Cl<sup>-</sup>

RN 760975-98-2 HCAPLUS  
 CN 1H-1,4-Diazepinium, 4-(4-amino-3-methylphenyl)hexahydro-1-methyl-1-[3-(1-pyrrolidiny)propyl]-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

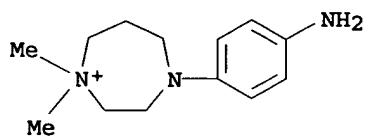
RN 760975-99-3 HCAPLUS  
 CN Piperazinium, 4-(4-amino-3-methylphenyl)-1-methyl-1-[3-(1-pyrrolidiny)propyl]-, chloride (9CI) (CA INDEX NAME)



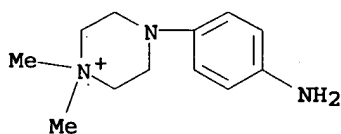
● Cl<sup>-</sup>

IT 760975-43-7P 760975-49-3P 760975-54-0P  
 RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (composition for dyeing of keratinic fibers comprising cationic derivative of phenylenediamine substituted by diazacyclohexane or diazacycloheptane)

RN 760975-43-7 HCAPLUS  
 CN 1H-1,4-Diazepinium, 4-(4-aminophenyl)hexahydro-1,1-dimethyl-, chloride (9CI) (CA INDEX NAME)

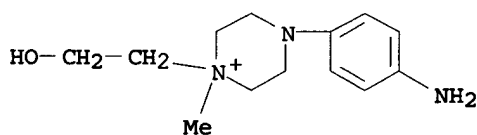
● Cl<sup>-</sup>

RN 760975-49-3 HCAPLUS  
 CN Piperazinium, 4-(4-aminophenyl)-1,1-dimethyl-, chloride,  
 dihydrochloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

●2 HCl

RN 760975-54-0 HCAPLUS  
 CN Piperazinium, 4-(4-aminophenyl)-1-(2-hydroxyethyl)-1-methyl-,  
 chloride, dihydrochloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

●2 HCl

IC ICM A61K007-13  
 ICS C07D243-08; C07D295-12  
 CC 62-3 (Essential Oils and Cosmetics)  
 Section cross-reference(s): 25  
 ST **hair dye** phenylenediamine diazacyclohexane  
 diazacycloheptane deriv  
 IT 760975-61-9 760975-63-1 760975-66-4  
 760975-68-6 760975-70-0 760975-72-2  
 760975-74-4 760975-76-6 760975-78-8  
 760975-80-2 760975-82-4 760975-83-5  
 760975-84-6 760975-85-7 760975-86-8

760975-87-9 760975-88-0 760975-89-1  
 760975-90-4 760975-91-5 760975-92-6  
 760975-93-7 760975-94-8 760975-95-9  
 760975-96-0 760975-97-1 760975-98-2  
 760975-99-3

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
 (composition for **dyeing** of **keratinic**  
**fibers** comprising cationic derivative of phenylenediamine  
 substituted by diazacyclohexane or diazacycloheptane)

IT 760975-43-7P 760975-49-3P 760975-54-0P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation); USES (Uses)

(composition for **dyeing** of **keratinic**  
**fibers** comprising cationic derivative of phenylenediamine  
 substituted by diazacyclohexane or diazacycloheptane)

IT 77-78-1, Methyl sulfate 5521-38-0 16155-03-6 223786-22-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(composition for **dyeing** of **keratinic**  
**fibers** comprising cationic derivative of phenylenediamine  
 substituted by diazacyclohexane or diazacycloheptane)

IT 760975-45-9P 760975-48-2P 760975-51-7P 760975-52-8P

760975-57-3P 760975-59-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)

(composition for **dyeing** of **keratinic**  
**fibers** comprising cationic derivative of phenylenediamine  
 substituted by diazacyclohexane or diazacycloheptane)

L52 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:133249 HCAPLUS

DOCUMENT NUMBER: 138:171819

TITLE: Composition for **dyeing**  
**keratinous fibers** containing  
 a p-phenylenediamine substituted by a  
 diazacycloheptane radical

INVENTOR(S): Sabelle, Stephane; Terranova, Eric

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------

WO 2003014093	A1	20030220	WO 2002-FR2822	
---------------	----	----------	----------------	--

2002  
0807

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA,  
 CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI,  
 GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,  
 KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK,  
 MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG,  
 SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,  
 ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT,  
 BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE,  
 IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM,  
 GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

FR 2828488	A1	20030214	FR 2001-10597	
------------	----	----------	---------------	--

2001  
0808

FR 2828488	B1	20050610		
------------	----	----------	--	--

EP 1417184	A1	20040512	EP 2002-772490	
------------	----	----------	----------------	--

2002  
0807

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,  
MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,  
EE, SK

JP 2005504046 T2 20050210 JP 2003-519043

2002  
0807

US 2005102769 A1 20050519 US 2003-485855

2002  
0807

PRIORITY APPLN. INFO.:

FR 2001-10597

A

2001  
0808

WO 2002-FR2822

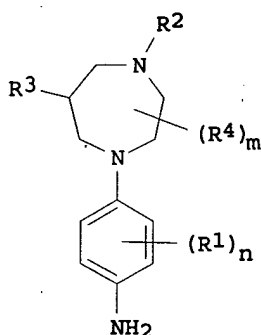
W

2002  
0807

OTHER SOURCE(S):

MARPAT 138:171819

GI



I

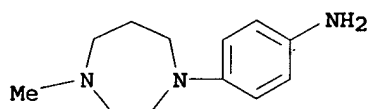
- AB The invention concerns a composition for oxidation dyeing of keratinous fibers, in particular human hair, comprising an oxidation base I [R<sub>1</sub> = halo, peroxide-, diazo-, NO<sub>2</sub>-, and NO-free (halo-substituted) C<sub>1</sub>-6 (cyclo) alkyl, optionally containing ≥1 of O, N, S, or SO<sub>2</sub>; n = 0-4; R<sub>2</sub> = H, (substituted) C<sub>4</sub>-7 alkyl, alkylcarbonyl, alkoxy carbonyl, mono- or dialkylcarbonyl, carbamoyl, or R<sub>6</sub>R<sub>7</sub>NC:NR<sub>5</sub>; R<sub>5</sub>-7 = H, C<sub>1</sub>-4 alkyl or hydroxyalkyl; R<sub>3</sub> = H, (unsatd.) alkyl, OH, hydroxyalkyl, alkoxy, alkoxyalkyl, alkylcarbonyl, hydroxyalkoxyalkyl, amino, mono- or dialkylamino, aminoalkyl, hydroxy(amino)alkyl, carboxy, carbamoyl, carbamoylalkyl, alkoxy carbonyl, or mono- or dialkylaminocarbonyl; R<sub>4</sub> = (unsatd.) alkyl, hydroxyalkyl, alkoxyalkyl, alkylcarbonyl, hydroxyalkoxyalkyl, aminoalkyl, hydroxy(amino)alkyl, carboxy, carboxyalkyl, carbamoyl, carbamoylalkyl, alkoxy carbonyl, or mono- or dialkylaminocarbonyl; m = 0-4] or their salts. The invention also concerns the method for dyeing keratinous fibers using said composition and the novel compds. mentioned above. Thus, I (R<sub>1</sub>, R<sub>3</sub>, R<sub>4</sub> = H, R<sub>2</sub> = Me) 2HCl was manufactured by reaction or 4-fluoronitrobenzene 5 h with 1-methyl[1,4]diazepane in water containing KCO<sub>3</sub> at 100, reduction of the intermediate in the presence of Pd/C and treatment of the reaction solution with HCl.
- IT 219132-82-8P, 1-Methyl-4-(4-aminophenyl)[1,4]diazepane  
497249-19-1P, 1-Methyl-4-(4-aminophenyl)[1,4]diazepane  
dihydrochloride 497249-23-7P 497249-27-1P

497249-28-2P, 4-(4-Aminophenyl)-1-methylcarbonyl[1,4]diazepane 497249-29-3P, 4-(4-Aminophenyl)[1,4]diazepane-1-carboximidamide 497249-30-6P, 4-(4-Aminophenyl)-N,N-dimethyl[1,4]diazepane-1-carboximidamide 497249-31-7P, 1-(4-Aminophenyl)-6-hydroxy-4-methyl[1,4]diazepane 497249-32-8P, 6-Amino-1-(4-aminophenyl)-4-methyl[1,4]diazepane 497249-33-9P, 1-(4-Aminophenyl)-6-hydroxy-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-34-0P, 6-Amino-1-(4-Aminophenyl)-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-35-1P, 1-(4-Aminophenyl)-6-hydroxy-4-(2-hydroxyethyl)[1,4]diazepane 497249-36-2P, 6-Amino-1-(4-Aminophenyl)-4-(2-hydroxyethyl)[1,4]diazepane 497249-37-3P, 1-(4-Aminophenyl)-4-(2-hydroxyethyl)-6-(hydroxymethyl)[1,4]diazepane 497249-38-4P, 2-Methyl-4-(4-methyl[1,4]diazepan-1-yl)phenylamine 497249-39-5P, 2-Methyl-4-[4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepan-1-yl]phenylamine 497249-40-8P, 1-(4-Amino-3-methylphenyl)-4-(2-hydroxyethyl)[1,4]diazepane 497249-41-9P, 1-(4-Amino-3-methylphenyl)-4-(methylcarbonyl)[1,4]diazepane 497249-42-0P, 4-(4-Amino-3-methylphenyl)[1,4]diazepane-1-carboximidamide 497249-43-1P, 4-(4-Amino-3-methylphenyl)-N,N-dimethyl[1,4]diazepane-1-carboximidamide 497249-44-2P, 1-(4-Amino-3-methylphenyl)-6-hydroxy-4-methyl[1,4]diazepane 497249-45-3P, 6-Amino-1-(4-amino-3-methylphenyl)-4-methyl[1,4]diazepane 497249-46-4P, 1-(4-Amino-3-methylphenyl)-6-hydroxy-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-47-5P, 6-Amino-1-(4-amino-3-methylphenyl)-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-48-6P, 1-(4-Amino-3-methylphenyl)-6-hydroxy-4-(2-hydroxyethyl)[1,4]diazepane 497249-49-7P, 6-Amino-1-(4-amino-3-methylphenyl)-4-(2-hydroxyethyl)[1,4]diazepane 497249-50-0P 497249-52-2P 497249-53-3P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(compns. containing p-phenylenediamines substituted by diazacycloheptane radicals for dyeing hair)

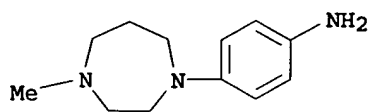
RN 219132-82-8 HCAPLUS

CN Benzenamine, 4-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)- (9CI)  
(CA INDEX NAME)



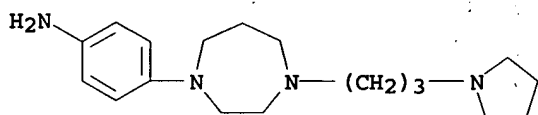
RN 497249-19-1 HCAPLUS

CN Benzenamine, 4-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-, dihydrochloride (9CI) (CA INDEX NAME)



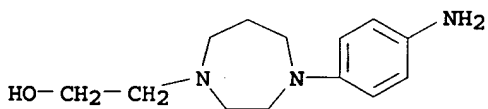
●2 HCl

RN 497249-23-7 HCAPLUS  
 CN Benzenamine, 4-[hexahydro-4-[3-(1-pyrrolidinyl)propyl]-1H-1,4-diazepin-1-yl]-, trihydrochloride (9CI) (CA INDEX NAME)



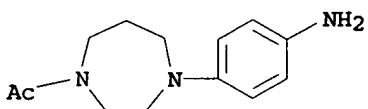
●3 HCl

RN 497249-27-1 HCAPLUS  
 CN 1H-1,4-Diazepine-1-ethanol, 4-(4-aminophenyl)hexahydro-, dihydrochloride (9CI) (CA INDEX NAME)



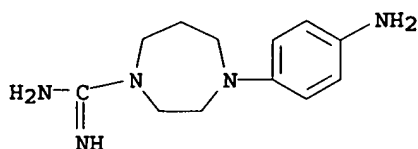
●2 HCl

RN 497249-28-2 HCAPLUS  
 CN 1H-1,4-Diazepine, 1-acetyl-4-(4-aminophenyl)hexahydro- (9CI) (CA INDEX NAME)

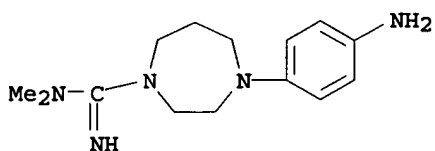


RN 497249-29-3 HCAPLUS  
 CN 1H-1,4-Diazepine-1-carboximidamide, 4-(4-aminophenyl)hexahydro- (9CI) (CA INDEX NAME)

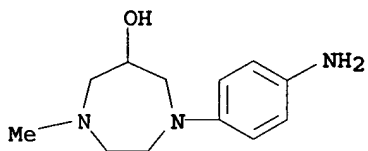




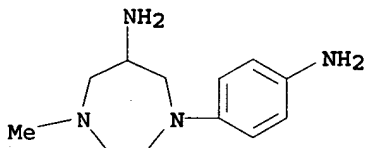
RN 497249-30-6 HCAPLUS  
 CN 1H-1,4-Diazepine-1-carboximidamide, 4-(4-aminophenyl)hexahydro-N,N-dimethyl- (9CI) (CA INDEX NAME)



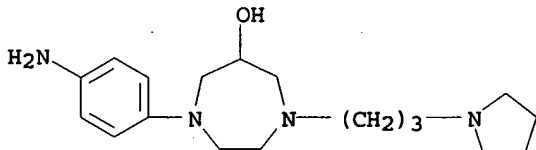
RN 497249-31-7 HCAPLUS  
 CN 1H-1,4-Diazepin-6-ol, 1-(4-aminophenyl)hexahydro-4-methyl- (9CI) (CA INDEX NAME)



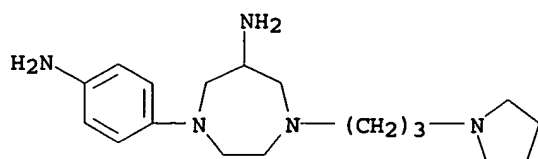
RN 497249-32-8 HCAPLUS  
 CN 1H-1,4-Diazepin-6-amine, 1-(4-aminophenyl)hexahydro-4-methyl- (9CI) (CA INDEX NAME)



RN 497249-33-9 HCAPLUS  
 CN 1H-1,4-Diazepin-6-ol, 1-(4-aminophenyl)hexahydro-4-[3-(1-pyrrolidinyl)propyl]- (9CI) (CA INDEX NAME)

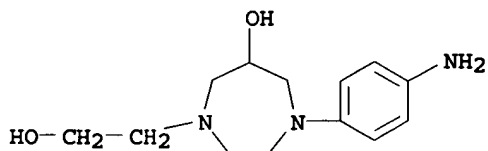


RN 497249-34-0 HCAPLUS  
 CN 1H-1,4-Diazepin-6-amine, 1-(4-aminophenyl)hexahydro-4-[3-(1-pyrrolidinyl)propyl]- (9CI) (CA INDEX NAME)



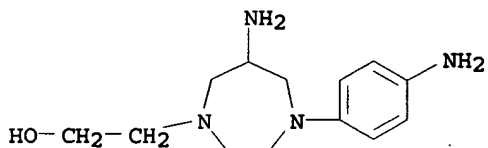
RN 497249-35-1 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanol, 4-(4-aminophenyl)hexahydro-6-hydroxy-  
(9CI) (CA INDEX NAME)



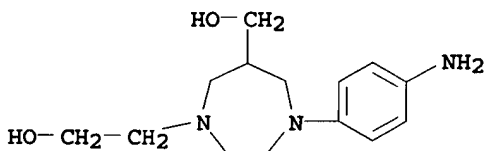
RN 497249-36-2 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanol, 6-amino-4-(4-aminophenyl)hexahydro-  
(9CI) (CA INDEX NAME)



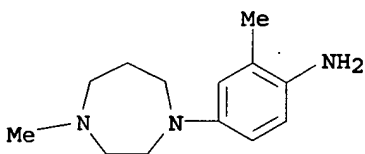
RN 497249-37-3 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanol, 4-(4-aminophenyl)hexahydro-6-  
(hydroxymethyl)- (9CI) (CA INDEX NAME)



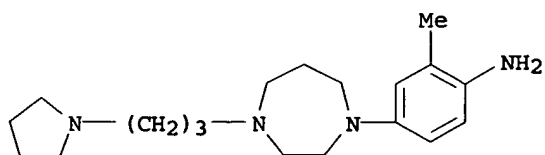
RN 497249-38-4 HCAPLUS

CN Benzenamine, 4-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-2-methyl-  
(9CI) (CA INDEX NAME)

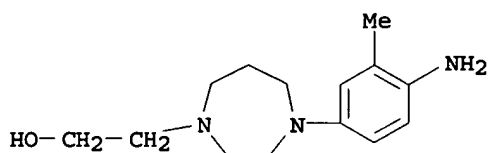


RN 497249-39-5 HCAPLUS

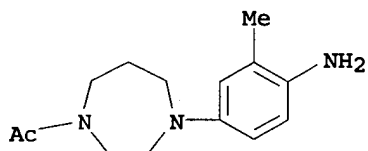
CN Benzenamine, 4-[hexahydro-4-[3-(1-pyrrolidinyl)propyl]-1H-1,4-  
diazepin-1-yl]-2-methyl- (9CI) (CA INDEX NAME)



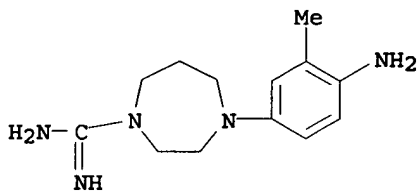
RN 497249-40-8 HCAPLUS  
 CN 1H-1,4-Diazepine-1-ethanol, 4-(4-amino-3-methylphenyl)hexahydro-  
 (9CI) (CA INDEX NAME)



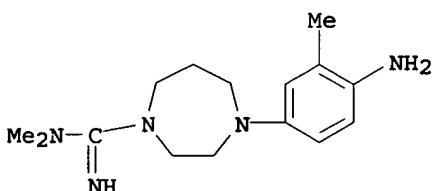
RN 497249-41-9 HCAPLUS  
 CN 1H-1,4-Diazepine, 1-acetyl-4-(4-amino-3-methylphenyl)hexahydro-  
 (9CI) (CA INDEX NAME)



RN 497249-42-0 HCAPLUS  
 CN 1H-1,4-Diazepine-1-carboximidamide, 4-(4-amino-3-methylphenyl)hexahydro- (9CI) (CA INDEX NAME)

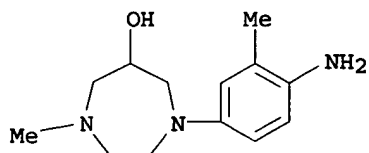


RN 497249-43-1 HCAPLUS  
 CN 1H-1,4-Diazepine-1-carboximidamide, 4-(4-amino-3-methylphenyl)hexahydro-N,N-dimethyl- (9CI) (CA INDEX NAME)



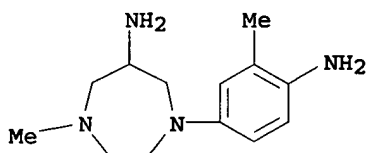
RN 497249-44-2 HCAPLUS

CN 1H-1,4-Diazepin-6-ol, 1-(4-amino-3-methylphenyl)hexahydro-4-methyl-  
(9CI) (CA INDEX NAME)



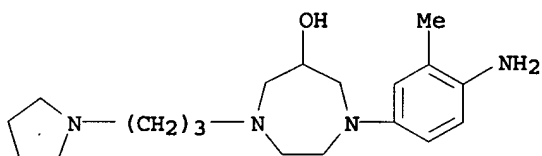
RN 497249-45-3 HCAPLUS

CN 1H-1,4-Diazepin-6-amine, 1-(4-amino-3-methylphenyl)hexahydro-4-methyl- (9CI) (CA INDEX NAME)



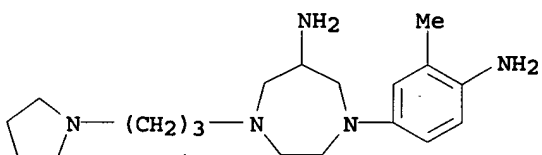
RN 497249-46-4 HCAPLUS

CN 1H-1,4-Diazepin-6-ol, 1-(4-amino-3-methylphenyl)hexahydro-4-[3-(1-pyrrolidinyl)propyl]- (9CI) (CA INDEX NAME)



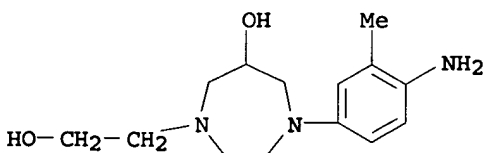
RN 497249-47-5 HCAPLUS

CN 1H-1,4-Diazepin-6-amine, 1-(4-amino-3-methylphenyl)hexahydro-4-[3-(1-pyrrolidinyl)propyl]- (9CI) (CA INDEX NAME)



RN 497249-48-6 HCAPLUS

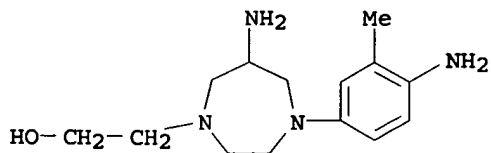
CN 1H-1,4-Diazepine-1-ethanol, 4-(4-amino-3-methylphenyl)hexahydro-6-hydroxy- (9CI) (CA INDEX NAME)



RN 497249-49-7 HCAPLUS

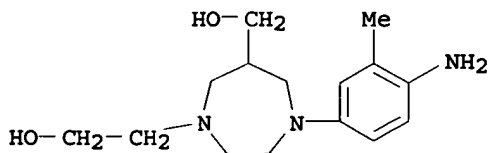
CN 1H-1,4-Diazepine-1-ethanol, 6-amino-4-(4-amino-3-

methylphenyl)hexahydro- (9CI) (CA INDEX NAME)



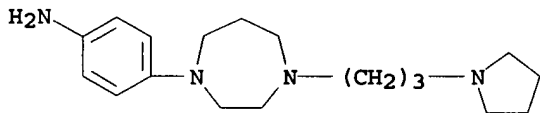
RN 497249-50-0 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanol, 4-(4-amino-3-methylphenyl)hexahydro-6-(hydroxymethyl)- (9CI) (CA INDEX NAME)



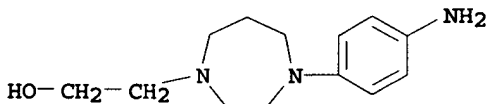
RN 497249-52-2 HCAPLUS

CN Benzenamine, 4-[hexahydro-4-[3-(1-pyrrolidinyl)propyl]-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)



RN 497249-53-3 HCAPLUS

CN 1H-1,4-Diazepine-1-ethanol, 4-(4-aminophenyl)hexahydro- (9CI) (CA INDEX NAME)



IC ICM C07D243-08

ICS A61K007-13

CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)

Section cross-reference(s): 28, 62

ST aminophenyldiazapane deriv hair dye;

methyldiazepanylphenylamine dye manuf hair

IT Hair preparations

(dyes; compns. containing p-phenylenediamines substituted by diazacycloheptane radicals for dyeing hair)

IT 219132-82-8P, 1-Methyl-4-(4-aminophenyl)[1,4]diazepane

497249-19-1P, 1-Methyl-4-(4-aminophenyl)[1,4]diazepane

dihydrochloride 497249-21-5P, 4-(4-Amino-3-

methylphenyl)[1,4]diazepane dihydrochloride 497249-23-7P

497249-25-9P, 1-(4-Aminophenyl)[1,4]diazepane dihydrochloride

497249-27-1P 497249-28-2P, 4-(4-Aminophenyl)-1-

methylcarbonyl[1,4]diazepane 497249-29-3P,

4-(4-Aminophenyl)[1,4]diazepane-1-carboximidamide

497249-30-6P, 4-(4-Aminophenyl)-N,N-dimethyl[1,4]diazepane-1-carboximidamide 497249-31-7P, 1-(4-Aminophenyl)-6-hydroxy-4-methyl[1,4]diazepane 497249-32-8P, 6-Amino-1-(4-aminophenyl)-4-methyl[1,4]diazepane 497249-33-9P, 1-(4-Aminophenyl)-6-hydroxy-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-34-0P, 6-Amino-1-(4-Aminophenyl)-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-35-1P, 1-(4-Aminophenyl)-6-hydroxy-4-(2-hydroxyethyl)[1,4]diazepane 497249-36-2P, 6-Amino-1-(4-Aminophenyl)-4-(2-hydroxyethyl)[1,4]diazepane 497249-37-3P, 1-(4-Aminophenyl)-4-(2-hydroxyethyl)-6-(hydroxymethyl)[1,4]diazepane 497249-38-4P, 2-Methyl-4-(4-methyl[1,4]diazepan-1-yl)phenylamine 497249-39-5P, 2-Methyl-4-[4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepan-1-yl]phenylamine 497249-40-8P, 1-(4-Amino-3-methylphenyl)-4-(2-hydroxyethyl)[1,4]diazepane 497249-41-9P, 1-(4-Amino-3-methylphenyl)-4-(methylcarbonyl)[1,4]diazepane 497249-42-0P, 4-(4-Amino-3-methylphenyl)[1,4]diazepane-1-carboximidamide 497249-43-1P, 4-(4-Amino-3-methylphenyl)-N,N-dimethyl[1,4]diazepane-1-carboximidamide 497249-44-2P, 1-(4-Amino-3-methylphenyl)-6-hydroxy-4-methyl[1,4]diazepane 497249-45-3P, 6-Amino-1-(4-amino-3-methylphenyl)-4-methyl[1,4]diazepane 497249-46-4P, 1-(4-Amino-3-methylphenyl)-6-hydroxy-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-47-5P, 6-Amino-1-(4-amino-3-methylphenyl)-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane 497249-48-6P, 1-(4-Amino-3-methylphenyl)-6-hydroxy-4-(2-hydroxyethyl)[1,4]diazepane 497249-49-7P, 6-Amino-1-(4-amino-3-methylphenyl)-4-(2-hydroxyethyl)[1,4]diazepane 497249-50-0P 497249-51-1P, 1-(4-Aminophenyl)[1,4]diazepane 497249-52-2P 497249-53-3P 497249-54-4P, 4-(4-Amino-3-methylphenyl)[1,4]diazepane

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(compns. containing p-phenylenediamines substituted by diazacycloheptane radicals for dyeing hair)

IT 108-45-2, m-Phenylenediamine, uses 108-46-3, m-Dihydroxybenzene, uses 591-27-5, m-Aminophenol 2835-95-2, 5-Amino-2-methylphenol 66422-95-5, 2,4-Diamino-1-(2-Hydroxyethoxy)benzene dihydrochloride  
RL: TEM (Technical or engineered material use); USES (Uses)  
(coupling agent; compns. containing p-phenylenediamines substituted by diazacycloheptane radicals for dyeing hair)

IT 220220-20-2P, 4-(3-Methyl-4-nitrophenyl)[1,4]diazepane 223786-22-9P, 1-Methyl-4-(4-nitrophenyl)[1,4]diazepane 497249-20-4P 497249-24-8P, 1-Benzyl-4-(4-nitrophenyl)[1,4]diazepane 497249-26-0P, 1-(2-Hydroxyethyl)-4-(4-nitrophenyl)[1,4]diazepane

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(dye precursor; compns. containing p-phenylenediamines substituted by diazacycloheptane radicals for dyeing hair)

IT 497249-22-6P, 1-(4-Nitrophenyl)-4-[3-(pyrrolidin-1-yl)propyl][1,4]diazepane

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(dye precursor; compns. containing p-phenylenediamines substituted by diazacycloheptane radicals for dyeing hair)

IT 350-46-9, 4-Fluoronitrobenzene 446-33-3, 4-Fluoro-2-methylnitrobenzene 4318-37-0, 1-Methyl[1,4]diazepane

4410-12-2, 1-Benzylhomopiperazine 53427-65-9,  
1-(2-Hydroxyethyl)homopiperazine 61903-11-5,  
1-Acetyl[1,4]diazepane 199475-39-3, 1-[3-(Pyrrolidin-1-yl)propyl]homopiperazine

RL: RCT (Reactant); RACT (Reactant or reagent)  
(dye precursor; compns. containing p-phenylenediamines  
substituted by diazacycloheptane radicals for dyeing  
hair)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L52 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:208250 HCAPLUS

DOCUMENT NUMBER: 134:252352

TITLE: Preparation of 3-aryl-2-  
aryluroidoalkylquinazolin-4-ones and related  
compounds as mediators of hedgehog signaling  
pathways.

INVENTOR(S): Baxter, Anthony David; Boyd, Edward Andrew;  
Guichert, Oivin M.; Price, Stephen; Rubin, Lee  
D.

PATENT ASSIGNEE(S): Curis, Inc., USA

SOURCE: PCT Int. Appl., 177 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019800	A2	20010322	WO 2000-US25461	2000 0915
WO 2001019800	A3	20011206		
WO 2001019800	C2	20021003		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2385736	AA	20010322	CA 2000-2385736	2000 0915
EP 1216234	A2	20020626	EP 2000-963551	2000 0915
EP 1216234	B1	20041229		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
JP 2003509414	T2	20030311	JP 2001-523380	2000 0915
US 6545005	B1	20030408	US 2000-663835	2000 0915
AT 286033	E	20050115	AT 2000-963551	2000 0915

EP 1516876	A1	20050323	EP 2004-28252	2000 0915
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AU 780846	B2	20050421	AU 2000-74948	2000 0915
ES 2234662	T3	20050701	ES 2000-963551	2000 0915
US 2005080138	A1	20050414	US 2004-953601	2004 0929
PRIORITY APPLN. INFO.:			US 1999-154526P	P 1999 0916
			US 1999-159412P	P 1999 1014
			US 1999-162899P	P 1999 1101
			EP 2000-963551	A3 2000 0915
			US 2000-663835	A2 2000 0915
			WO 2000-US25461	W 2000 0915
			US 2000-687800	B2 2000 1013
			US 2000-711343	B2 2000 1109
			US 2000-724277	A1 2000 1128

## OTHER SOURCE(S): MARPAT 134:252352

AB R1LX1Y1Z1LX2Y2Z2LR2 [R1, R2 = H, alkyl, (substituted) aryl, aralkyl, heteroaryl, heteroarylalkyl; L = null, alkyl, alkenyl, alkynyl, (CH<sub>2</sub>)<sub>n</sub>O(CH<sub>2</sub>)<sub>p</sub>, etc.; n, p = 0-10; X1, X2 = NR<sub>8</sub>, O, S, Se, N:N, ON:CH, heterocyclyl, bond, etc.; Y1, Y2 = CO, CS, SO<sub>2</sub>, SO, C(:NCN), heteroaryl, bond, etc.; Z1, Z2 = NR<sub>8</sub>, O, S, Se, N:N, ON:CH, heterocyclyl, bond, etc.; R<sub>8</sub> = H, alkyl, (substituted) aryl, aralkyl, heteroaryl, heteroaralkyl, etc.], were prepared Thus, triphosgene in EtOAc was added to 4-nitro-3-trifluoromethylaniline in EtOAc followed by stirring and reflux. The mixture was concentrated, dissolved in CHCl<sub>3</sub>, and treated with 3-(4-fluorophenyl)-2-(1-methylaminoethyl)-4-oxo-3,4-dihydroquinazoline in CHCl<sub>3</sub> to give 97% 1-[1-[3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl]ethyl]-3-(3-trifluoromethyl-4-nitrophenyl)-1-methylurea. The latter inhibited sonic hedgehog-induced Gli transcription activity with IC<sub>50</sub> <5 μM.

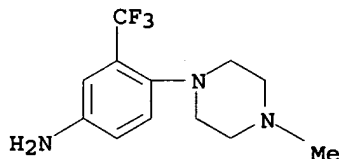


IT 330796-48-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of 3-aryl-2-aryluroidoalkylquinazolin-4-ones and  
 related compds. as mediators of hedgehog signaling pathways)

RN 330796-48-0 HCAPLUS

CN Benzenamine, 4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)- (9CI)  
 (CA INDEX NAME)



IC ICM C07D239-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 62

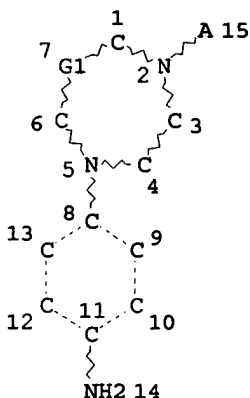
IT 74-89-5, Methylamine, reactions 111-95-5 118-92-3, Anthranilic  
 acid 123-62-6, Propionic anhydride 134-20-3, Methyl  
 anthranilate 329-01-1, 3-Trifluoromethylphenyl isocyanate  
 349-65-5, 2-Methoxy-5-trifluoromethylaniline 371-40-4,  
 4-Fluoroaniline 393-11-3, 4-Nitro-3-trifluoromethylaniline  
 426-59-5, 3-Aminophenyl trifluoromethyl sulfone 777-44-6,  
 3-Trifluoromethylphenylsulfonyl chloride 1138-80-3 2251-65-2,  
 3-Trifluoromethylbenzoyl chloride 5345-47-1, 2-Aminonicotinic  
 acid 39920-37-1, 2,6-Dichlorophenyl isocyanate 92511-32-5  
 330796-47-9 330796-48-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 3-aryl-2-aryluroidoalkylquinazolin-4-ones and  
 related compds. as mediators of hedgehog signaling pathways)

=&gt; =&gt; d que stat 148

L7 STR



REP G1=(0-1) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

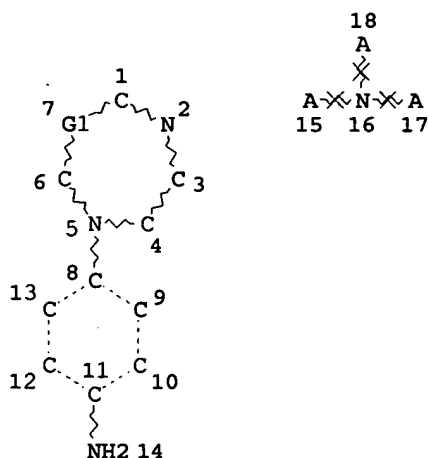
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L9 846 SEA FILE=REGISTRY SSS FUL L7

L11

STR

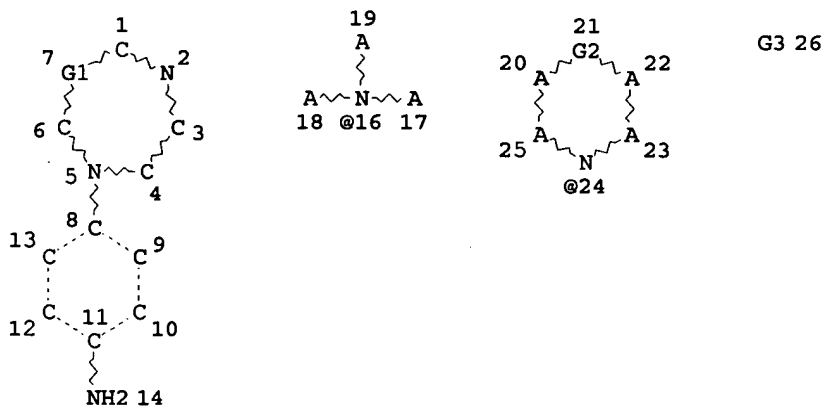


REP G1=(0-1) C  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L13 207 SEA FILE=REGISTRY SUB=L9 SSS FUL L11  
 L28 STR



REP G1=(0-1) C  
 REP G2=(0-1) A  
 VAR G3=16/24  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L30 243 SEA FILE=REGISTRY SUB=L9 SSS FUL L28  
 L45 1 SEA FILE=CAOLD ABB=ON PLU=ON L13  
 L46 2 SEA FILE=CAOLD ABB=ON PLU=ON L30

L47 6 SEA FILE=CAOLD ABB=ON PLU=ON L9  
 L48 6 SEA FILE=CAOLD ABB=ON PLU=ON (L45 OR L46 OR L47)

=> d 148 1-6 all hitstr

L48 ANSWER 1 OF 6 CAOLD COPYRIGHT 2006 ACS on STN

AN CA64:12852g CAOLD

TI diazonium salts (light-sensitive)

PA General Aniline & Film Corp.

DT Patent

PATENT NO.	KIND	DATE
NL 6505812		
BE 663606		
FR 1441795		
5521-23-3	5521-24-4	5521-25-5
5521-28-8	5521-29-9	5521-38-0
6826-94-4	17030-18-1	17069-23-7
17099-46-6	17099-47-7	94786-00-2
98001-18-4	98924-29-9	

PI NL 6505812

BE 663606

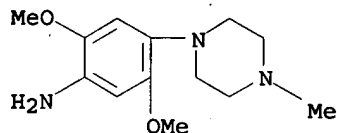
FR 1441795

IT 5521-23-3	5521-24-4	5521-25-5	5521-26-6	5521-27-7
5521-28-8	5521-29-9	5521-38-0	5521-39-1	
6826-94-4	17030-18-1	17069-23-7	17099-39-7	17099-43-3
17099-46-6	17099-47-7	94786-00-2	96279-22-0	97785-12-1
98001-18-4	98924-29-9			

IT 5521-27-7 5521-39-1

RN 5521-27-7 CAOLD

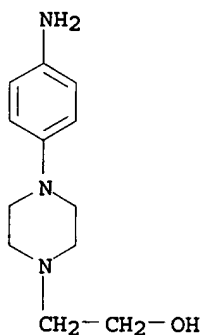
CN Piperazine, 1-(4-amino-2,5-dimethoxyphenyl)-4-methyl-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)



●2 HCl

RN 5521-39-1 CAOLD

CN 1-Piperazineethanol, 4-(4-aminophenyl)- (9CI) (CA INDEX NAME)



L48 ANSWER 2 OF 6 CAOLD COPYRIGHT 2006 ACS on STN

AN CA64:6534h CAOLD

TI preparative routes to tertiary amine-substituted nitroanilines

AU Ainsworth, D. P.; Suschitzky, H.

TI ylide methylation of aromatic nitro compds.

AU Traynelis, Vincent J.; McSweeney, J. V.

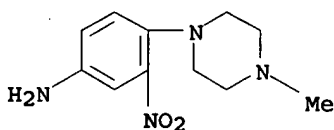
IT 81-20-9	83-41-0	83-42-1	881-03-8	1138-83-6
1890-33-1	3412-44-0	3487-44-3	4031-79-2	4031-80-5

4837-88-1	5355-60-2	5367-24-8	5367-26-0	5367-28-2
5367-32-8	5367-35-1	5367-36-2	5367-37-3	5367-38-4
5367-39-5	5367-40-8	5367-41-9	5367-42-0	5367-43-1
5367-44-2	5367-45-3	5367-46-4	5367-47-5	5367-48-6
5367-49-7	5367-51-1	5367-52-2	5367-53-3	5367-54-4
5367-55-5	5367-56-6	5367-57-7	5367-58-8	5367-59-9
5367-60-2	5367-61-3	5367-62-4	5367-64-6	5367-65-7
5367-66-8	5367-67-9	5367-68-0	5367-69-1	
5367-70-4	5367-71-5	5367-72-6	5381-75-9	5381-76-0
5381-77-1	5381-78-2	5381-79-3	5381-80-6	5381-81-7
5381-82-8	5565-57-1	5991-09-3		

IT 5367-67-9

RN 5367-67-9 CAOLD

CN Piperazine, 1-(4-amino-2-nitrophenyl)-4-methyl- (7CI, 8CI) (CA INDEX NAME)



L48 ANSWER 3 OF 6 CAOLD COPYRIGHT 2006 ACS on STN

AN CA62:11830e CAOLD

TI 1,4-disubstituted piperazines

AU Tomcufcik, Andrew S.; Fabio, P. F.; Hoffman, A. M.

DT Patent

TI piperazines (1,4-disubstituted)

PA American Cyanamid Co.

DT Patent

PATENT NO.	KIND	DATE
------------	------	------

PI BE 637271

GB 1047935

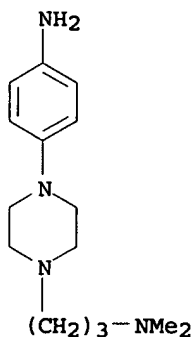
NL 297170

IT	148-84-5	298-78-2	299-48-9	299-54-7	710-17-8
	717-09-9	725-20-2	725-21-3	729-21-5	729-22-6
	729-93-1	732-78-5	733-20-0	735-70-6	738-19-2
	739-80-0	739-81-1	739-90-2	739-91-3	740-71-6
	741-91-3	743-73-7	743-74-8	744-00-3	744-40-1
	747-11-5	747-83-1	787-74-6	790-27-2	790-28-3
	794-85-4	794-86-5	794-90-1	796-92-9	796-98-5
	803-78-1	831-37-8	837-52-5	842-59-1	847-41-6
	849-77-4	851-89-8	852-51-7	859-40-5	877-96-3
	881-80-1	891-27-0	895-38-5	895-39-6	895-68-1
	897-93-8	900-57-2	901-97-3	902-03-4	907-48-2
	907-95-9	909-23-9	954-51-8	954-52-9	959-15-9
	961-85-3	961-92-2	967-76-0	970-97-8	971-69-7
	973-70-6	980-77-8	980-90-5	985-49-9	985-76-2
	988-90-9	1029-78-3	1030-53-1	1037-14-5	1041-12-9
	1041-76-5	1041-77-6	1046-92-0	1052-42-2	1052-66-0
	1057-17-6	1057-67-6	1057-82-5	1061-14-9	1063-52-1
	1095-51-8	1096-81-7	1102-29-0	1105-60-8	1105-86-8
	1149-37-7	1157-77-3	1164-06-3	1177-02-2	1233-12-1
	1244-61-7	1252-69-3	1252-78-4	1254-46-2	1257-51-8
	1923-93-9	3269-80-5	3317-93-9	3317-94-0	3428-27-1
	3441-98-3	12005-09-3	91954-38-0	93140-48-8	93147-28-5
	93480-11-6	97598-08-8	101034-41-7		

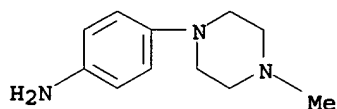
IT 790-27-2

RN 790-27-2 CAOLD

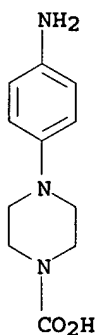
CN 1-Piperazinepropanamine, 4-(4-aminophenyl)-N,N-dimethyl- (9CI)  
(CA INDEX NAME)



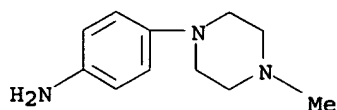
L48 ANSWER 4 OF 6 CAOLD COPYRIGHT 2006 ACS on STN  
 AN CA60:15868h CAOLD  
 TI synthesis of thiourea derivs. - (III) piperazinythiocarbanilides  
 and arylthiocarbamoylpiperazines  
 AU Galstukhova, N. B.; Shchukina, M. N.  
 IT 16153-81-4 16155-03-6 28439-90-9 28439-91-0  
 34349-88-7 89169-35-7 89169-36-8 91643-97-9 91646-66-1  
 93023-56-4 94264-50-3 94438-24-1 94520-33-9  
 95443-43-9 96766-17-5 98363-81-6 98845-39-7 99870-22-1  
 100302-40-7 100576-48-5 100623-85-6 101632-43-3 103192-78-5  
 IT 16153-81-4 91646-66-1 94520-33-9  
 RN 16153-81-4 CAOLD  
 CN Benzenamine, 4-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 91646-66-1 CAOLD  
 CN 1-Piperazinecarboxylic acid, 4-(p-aminophenyl)- (7CI) (CA INDEX NAME)

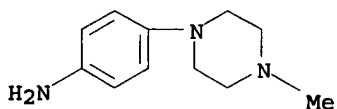


RN 94520-33-9 CAOLD  
 CN Benzenamine, 4-(4-methyl-1-piperazinyl)-, hydrochloride (9CI) (CA INDEX NAME)



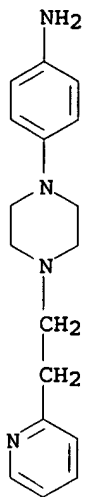
●x HCl

L48 ANSWER 5 OF 6 CAOLD COPYRIGHT 2006 ACS on STN  
 AN CA59:15271c CAOLD  
 TI ethylenimine-2-carbanilides and isomeric 3-pyridazolidones thereof  
 AU Wagner-Jauregg, Theodor; Zirngibl, L.  
 IT 3490-67-3 5369-34-6 10220-22-1 16153-81-4  
 16155-03-6 18606-63-8 27301-73-1 29425-96-5 35197-07-0  
 35216-60-5 41838-46-4 48128-18-3 88564-45-8 88564-46-9  
 88564-64-1 88637-09-6 88858-05-3 88858-06-4 89673-65-4  
 89774-20-9 89895-41-0 90002-84-9 90087-54-0 90205-35-9  
 90841-17-1 90875-41-5 90950-55-3 90972-71-7 91211-59-5  
 91335-99-8 91346-62-2 91355-91-8 91370-38-6 91370-39-7  
 91494-52-9 91564-99-7 92018-74-1 92036-73-2 92040-46-5  
 92041-46-8 92298-63-0 92317-64-1 92320-41-7 92320-53-1  
 92326-48-2 92653-56-0 92698-65-2 92727-92-9 92848-98-1  
 93089-00-0 93141-88-9 93161-02-5 93310-55-5 93540-86-4  
 93719-26-7 93719-38-1 94163-63-0 94165-66-9 94262-01-8  
 94262-04-1 94262-05-2 94296-97-6 94432-13-0 94907-65-0  
 94913-15-2 95423-99-7 95427-65-9 95428-64-1 95485-88-4  
 97281-78-2 97281-81-7 97493-52-2 97493-53-3 97554-49-9  
 97593-98-1 98250-56-7 99282-21-0 100022-94-4 100260-72-8  
 102287-47-8 106479-47-4 112001-14-6  
 IT 16153-81-4  
 RN 16153-81-4 CAOLD  
 CN Benzenamine, 4-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

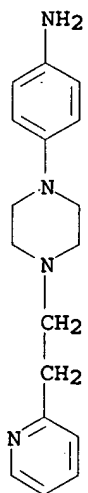


L48 ANSWER 6 OF 6 CAOLD COPYRIGHT 2006 ACS on STN  
 AN CA57:16634e CAOLD  
 TI fluorubin  
 AU Deuschel, Werner; Vilsmeier, W.; Riedel, G.  
 PA Badische Anilin- & Soda-Fabrik A.-G.  
 DT Patent  
 PATENT NO. KIND DATE  
 -----  
 PI BE 612092  
 DE 1149477  
 GB 1008467  
 IT 3965-85-3 3965-87-5 6640-47-7 34117-90-3 54940-73-7  
 66711-34-0 66711-35-1 91974-55-9 93437-35-5  
 93726-23-9 94383-30-9 94710-05-1 94804-40-7  
 94995-76-3 94995-77-4 95865-93-3 95866-01-6 97362-07-7  
 97435-94-4 97594-43-9 97737-56-9 97753-99-6 97979-19-6  
 97999-90-1 98000-59-0 98132-22-0 98339-12-9 98339-13-0  
 98339-14-1 98339-15-2 99872-19-2  
 IT 93437-35-5 94710-05-1  
 RN 93437-35-5 CAOLD  
 CN Piperazine, 1-(p-aminophenyl)-4-[2-(2-pyridyl)ethyl]- (7CI) (CA

INDEX NAME)



RN 94710-05-1 CAOLD  
CN Piperazine, 1-(p-aminophenyl)-4-[2-(2-pyridyl)ethyl]-,  
trihydrochloride (7CI) (CA INDEX NAME)



● 3 HCl

=&gt;